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# VARIATIONAL ENERGY PRINCIPLE FOR COMPRESSIBLE, BAROCLINIC FLOW II. FREE-ENERGY FORM OF HAMILTON'S PRINCIPLE



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## II. FREE-ENERGY FORM OF HAMILTON'S PRINCIPLE

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## ABSTRACT

The first and second variations are calculated for the irreducible form of Hamilton's Principle that involves the minimum number of dependent variables necessary to describe the kinematics and thermodynamics of inviscid, compressible, baroclinic flow in a specified gravitational field. The form of the second variation shows that, in the neighborhood of a stationary point that corresponds to physically stable flow, the action integral is nevertheless a complex saddle-surface in parameter space. Thus it would be extremely difficult to solve a problem by minimizing this action integral. There exists, however, an alternative form of Hamilton's Principle for which such a direct solution of a flow problem is possible. This second form is related to the first by a Friedrichs transformation of the thermodynamic variables. This introduces an extra dependent variable, but the first and second variations are shown to have direct physical significance, namely they are equal to the free energy of fluctuations about the equilibrium flow that satisfies the equations of motion. If this equilibrium flow is physically stable, and if a very weak second-order integral constraint on the correlation between the fluctuations of otherwise independent variables is satisfied, then the second variation of the action integral for this free-energy form of Hamilton's Principle is positive-definite, so the action integral is a minimum, and can serve as the basis for a direct trial-and-error solution. The second-order integral constraint states that the unavailable energy must be maximum at equilibrium, i.e. the fluctuations

must be so correlated as to produce a second-order decrease in the total unavailable energy. In a numerical calculation this constraint is easy to impose, but its effect in most problems is so weak that it can be ignored altogether. The free-energy form of Hamilton's Principle has the further advantage that it allows easy handling of the free-boundary problem.

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## II. FREE-ENERGY FORM OF HAMILTON'S PRINCIPLE

## I. INTRODUCTION AND SUMMARY

At the beginning of the preceding paper (which will be referred to as Paper I) it was remarked that the goal of these papers is to develop a variational energy principle that will be suitable for direct (i.e. trial-and-error) solutions of fluid flow problems. For this purpose it is necessary that, at least in the case of physically stable flows, the action integral whose minimization serves as the basis of the calculational procedure must indeed be a **minimum**, rather than a saddle point, for the desired solution that satisfies the equations of motion. In order to test whether a given action integral has this property, it is necessary to calculate its second variation. The mathematics necessary to do this was developed in Paper I, in which boundary and terminal conditions were also discussed in detail, as was the connection between physical stability and the curvature properties (i.e. the sign of the second variation) of an action integral that can be interpreted as the time-average total free energy of the fluid system.

In this paper it will be shown that such an action integral does in fact exist. This is demonstrated (in Section VII A) by carrying out an explicit calculation of the first and second variations, and showing that the necessary condition for the vanishing of the first variation is the fulfillment of the known equations of motion, and that the second variation is indeed equal to the second-order change in the free energy that is associated with fluctuations in the fluid.

In order to be able to identify the various terms in the second variation with the various types of displacement and compression work in a stratified atmosphere and with the changes in unavailable energy that are associated with entropy fluctuations, a great deal of preliminary discussion, given in Section II, is necessary. In Section II C a generalization of the buoyancy displacement work is derived that does not assume either that the volume of the displaced sample of fluid remains constant (Boussinesq approximation), or that it adjusts itself so that the internal pressure is always equal to the local external pressure (Väisälä-Brunt approximation). Rather, the generalized expression allows for a completely arbitrary volume change, which physically corresponds to the case of fast spontaneous displacements in which inertial forces corresponding to internal turbulence within the sample account for the difference between the internal and external pressures. Sections II B, D, E, and F treat various aspects of the use of dual state functions to describe the fluctuations about equilibrium that occur in a turbulent fluid. This involves interpreting the inequality that is satisfied by dual molar internal energy functions in terms of a fluctuating entropy density. This inequality constitutes a statement of the Second Law of Thermodynamics. The generalization of this basic thermodynamic inequality from a homogeneous fluid at rest to a compressible fluid in an arbitrary state of motion is shown in Section VII E to be equivalent to the corresponding inequality that is satisfied by the free-energy form of Hamilton's Principle.

The important thermodynamic issues involved in the variational treatment of fluid motion come to light already in the static case of fluctuations about hydrostatic equilibrium in a stratified atmosphere. It is shown in Sections IV and V that two different variational energy principles exist for a static atmosphere. The first is the well-known statement[1] that at equilibrium the total potential energy E (i.e. the sum of the internal thermal energy and the gravitational energy) is minimum. The proof of this that is given in Section IV,

unlike the one available in the literature,[1] does not make use of non-holonomic differential expressions, but rather is based on a direct calculation of the first and second variations of an explicitly defined integral functional for the total energy of the atmosphere.

The second variational energy principle, which is discussed in Section V, is the statement that at equilibrium the total free energy A of a static atmosphere is minimum. The free energy in question is the available energy of the non-equilibrium fluctuations, and its introduction is not simply a matter of replacing the thermodynamic internal energy with the Helmholtz or Gibbs functions, since both of these refer to equilibrium conditions. Rather, it is necessary to demonstrate by explicit calculation that the first and second variations of the integral functional that is alleged to represent the total free energy of the fluctuating atmosphere do in fact have the form of a change in free energy, namely the work performed minus the increase in unavailable energy. The equilibrium value $\tilde{A}$ of the total free potential energy can be adjusted to any desired value by means of an additive constant. The choice of constant made in this paper is such that $\tilde{A} = -\tilde{E}$. With this choice, the principles based on E and A are related to each other through a Friedrichs transformation,[2] and can be used in concert to give a minimax description of a static atmosphere that is the analog of the well-known minimax description of static elastic structures that is a consequence of the Friedrichs transformation.

The two variational minimum principles for a static atmosphere can be regarded as dual adaptations of the Principle of Virtual Work to a continuum. This approach is discussed in Section III where it is noted that these dual principles of virtual work are equivalent to the two competing approaches to elastic structures that are embodied in the principles of Dirichlet and Castigliano.[3]

The two alternative variational minimum principles for a static atmosphere can both be adapted to an atmosphere in motion by including kinetic energy in the action integral. This leads to two different forms of Hamilton's Principle depending on whether the potential energy is represented by the total energy E or by the free energy A. The first case, which is discussed in Section VI, has the advantage of involving the minimum possible number of dependent variables, and so is called the **irreducible form** of Hamilton's Principle. It has the great disadvantage, however, that the integrand of the action integral, which is the **difference** of kinetic and potential energy, is not a physically meaningful energy. This is reflected in the fact that the second variation of the irreducible form of Hamilton's Principle is indefinite in sign, which means that the action surface in parameter space (i.e. the plot of the action integral as a function of all the adjustable parameters involved in the trial functions) is an intricate saddle-surface at the stationary point representing flow that obeys the equations of motion. This means that any attempt to "home-in" on this point by successive iterations of the parameters chosen so as to decrease the value of the action integral would almost certainly be doomed to failure.

The dual form of Hamilton's Principle that results when the potential energy is represented by the free energy A is called the **free-energy form** of Hamilton's Principle, and is discussed in Section VII. In addition to the dependent variables involved in the irreducible form of the principle, the free-energy form involves the molar enthalpy H. This extra degree of freedom makes it possible to describe fluctuations in molar entropy S about the specified average value. The great advantage of the free energy form of Hamilton's Principle is that the action integral is the time integral of the **sum** of the kinetic and free potential energy, and so (when divided by the total time interval) can be interpreted as the time-average of the **total free energy** of the fluid system. This is reflected in the fact that the second variation has the form of the total second-order change in kinetic and potential

energy minus the increase in unavailable energy that results from the fluctuation in entropy (which is represented indirectly through the flucutations in the enthalpy and pressure). Thus the fluctuations in the dependent variables faithfully generate the fluctuations in total free energy that occur in a turbulent fluid. One physical feature that the mathematics does not automatically duplicate is the subtle kind of correlation that results between the otherwise independent fluctuations in enthalpy and particle displacement because of the Second Law. This is a very weak second-order constraint that requires that a certain space-time integral (Eq. (120b)) involving products of the otherwise independent fluctuations must be non-negative. When this constraint is satisfied, the second variation of the free-energy form of Hamilton's Principle is positive-definite if the flow is physically stable, and this fact means that its action integral can be used as the basis for a direct solution of flow problems. The Second-Law constraint must be imposed on the successive changes in the parameters only in the neighborhood of an extremum where the second variation is comparable in magnitude to the first variation. There are several ways in which this can easily be done, but for most problems it should be possible to ignore the constraint altogether. These matters are discussed in greater detail in Section VII F.

The free-energy form of Hamilton's Principle has the further important advantage that it is very well suited to **free-boundary** problems. This feature, which is closely related to the well-known advantage of the Castigliano Principle over the Dirichlet Principle in fitting boundary conditions when loads rather than deflections are specified, is discussed in Section VII B.

Aside from its utility for direct solutions, the free-energy form of Hamilton's Principle provides an efficient way of deriving sufficient criteria for stability. This is illustrated in Section VII D by a derivation of the well-known criterion[4, 5] for buoyancy stability of a shearing wind.

The construction of the free-energy form of Hamilton's Principle amounts to the extension of thermodynamic formalism and methodology to a heterogeneous continuum in an arbitrary state of motion. It is pointed out in Sections VII E and VIII that this suggests some possibly fruitful new approaches to the problems of fluid dynamics and dynamical meteorology.

A brief survey of the literature relevant to variational principles for a fluid is given in the Appendix.

**Notation**

The notation of Paper I will be continued. In general, lower case letters will be used for densities of extensive quantities (such as the mole density n), and ordinary capitals will designate either molar quantities (such as the molar entropy S), or intensive quantities (such as the temperature T). Sans serif capitals will designate total extensive quantities (such as total volume V). To avoid confusion with the fluid speed $V \equiv (V \cdot V)^{1/2}$, molar volume will be designated by $\hat{V}$. Because the letter W has already been assigned to kinetic energy, work (Arbeit) will be designated by $\delta A$. Since free-energy is just the work function, A will also represent the molar free potential energy. A script capital will represent either the bounding surface $\mathscr{S}$, the molar deformation force $\mathscr{D}$, or a total action $-\mathscr{L}$ for the irreducible form of Hamilton's Principle, and $\mathscr{A}$ for the free-energy form.

## II. PRELIMINARIES

### A. Equations of Motion

The necessary kinematical relations have been given in Section II of Paper I. In a **convected-frame** treatment, the trial functions give the three components of the position vector $\mathbf{X}(\Lambda, t)$. (When used as an argument or subscript, $\Lambda^A$ will usually be indicated simply as $\Lambda$.) The molar volume $\hat{V}$ and the velocity $\mathbf{V}$ are given by

$$\hat{V} = \det\left(\frac{\partial X^j}{\partial \Lambda^A}\right) \equiv J^X_\Lambda \; ; \; \mathbf{V} = \left(\frac{\partial \mathbf{X}}{\partial t}\right)_\Lambda \equiv D_t \mathbf{X} \qquad (1a, b)$$

where $J^X_\Lambda$ and $D_t$ are used to designate the Jacobian and the material time derivative respectively.

In an **inertial-frame** treatment, the trial functions give the space-time dependence of the three families of Lagrange surfaces $\Lambda^A(\boldsymbol{x}, t)$. The mole density $n = \hat{V}^{-1}$, the material time derivative, and the velocity are given by

$$n = J^\Lambda_{\boldsymbol{x}} = (\nabla\Lambda^1) \cdot (\nabla\Lambda^2 \times \nabla\Lambda^3) \; ; \; D_t = \partial_t + \mathbf{V} \cdot \nabla \; ; \qquad (2a, b)$$

$$\mathbf{V} = -\sum_{A=1}^{3} (\partial_t \Lambda^A)(\nabla\Lambda^B \times \nabla\Lambda^C)/n \; ; \; (A, B, C \text{ cyclic}) \qquad (2c)$$

where $\partial_t$ is the partial with time at a fixed $\boldsymbol{x}$-position.

It was pointed out in Equation (20) of Paper I that in the Lagrange kinematics the conservation equation is identically satisfied, so this need not be included among the equations of motion.

For reversible adiabatic flow, the local energy equation reduces to the statement that molar entropy is a constant of motion. In the Lagrange kinematics used here, this requirement is very easily satisfied by specifying the molar entropy S to be the appropriate

function of the Lagrange parameters $\Lambda^A$. In a convected-frame treatment, the specified function $S(\Lambda^A)$ has no variation. The same is true if $S = S(\Lambda^A, t)$ is a specified function of the time as well as of $\Lambda^A$. Allowing S to be time-dependent provides a way of introducing a specified diabatic heating into the formalism. Thus, in a convected-frame treatment

$$S = S(\Lambda^A, t) = \text{specified function} ; \tag{3a}$$

$$\delta^{(1+2)}S = 0 . \text{ (Convected Frame)} \tag{3b}$$

In an inertial-frame treatment, the fact that $\delta\Lambda^A \neq 0$ means that $\delta S \neq 0$. The expression for this variation was given in Equation (43) of Paper I:

$$S = S[\Lambda^A(\boldsymbol{x}, t); t] \text{ ; (Inertial Frame)} \tag{4a}$$

$$\delta^{(1+2)}S = \delta\Lambda^A(\overline{\partial_A S}) + \tfrac{1}{2}\delta\Lambda^A\delta\Lambda^B(\overline{\partial_A \partial_B S}) \tag{4b}$$

$$= -\delta\mathbf{X} \cdot \nabla\bar{S} + \tfrac{1}{2}(\delta\mathbf{X}\delta\mathbf{X}:\nabla\nabla\bar{S}) . \tag{4c}$$

The simplest way of representing the pressure p is as a known function of $\hat{V}$ (or n) and S. (An alternative representation will be introduced in Subsection D below.) Thus

$$p = p(\hat{V}, S) \equiv -(\partial U/\partial\hat{V})_S \tag{5}$$

which follows from the expression for the first differential of the canonical molar internal energy state function $U(S, \hat{V})$:

$$dU = TdS - pd\hat{V} \tag{6}$$

where T is the absolute temperature. Equations (5) and (6) are appropriate for a convected-frame treatment. In an inertial-frame treatment, the appropriate canonical state function is the internal energy **density** $u(S, n)$ for which

$$du = nTdS + Hdn \tag{7}$$

where H is the molar enthalpy. The pressure function $p = p(n, S)$ is defined in terms $u(S, n)$ as follows:

$$p \equiv nH - u = n(\partial u/\partial n)_S - u . \tag{8}$$

Thus p is derived from $u$ by a Legendre transformation, and so the two are dual state functions.

It should be noted parenthetically that the thermodynamic treatment developed in this paper is a truncated version of a more complete and more symmetric treatment[6] that is based on $u(\mathfrak{s}, n)$, where $\mathfrak{s}$ is the entropy **density**, rather than the molar entropy S. The present treatment has the advantage of the greater simplicity that results from specifying the functional form of $S(\Lambda, t)$ in advance. The more complete theory is necessary, however, in fluid problems involving either different chemical constituents, or different phases of a single constituent.

Since the mass conservation and the energy equations are identically satisfied, the only equation of motion that remains to be satisfied is the statement of local conservation of momentum. For inviscid flow this is Euler's equation:

$$M\tilde{D}_t\tilde{V} = -\frac{1}{\tilde{n}}\nabla\tilde{p} - M\nabla\tilde{\phi} \tag{9}$$

where $\phi = \phi(\mathbf{x}, t)$ is the given gravitational potential. The tilde has been added to emphasize that this equation is satisfied by **equilibrium flow**, i.e. flow for which the local force balance is everywhere maintained. In a variational context, this corresponds to the **extremal flow** for which the first variation of the action integral vanishes.

Non-extremal flows can be represented by adding a "deformation" or "displacement" force $\mathcal{F}$ to the right-hand side of Equation (9). This then represents the effective force field that would have to be added in order to maintain the force balance (or conservation of momentum) of an arbitrarily specified flow. The work associated with the imposition of such a force field is discussed in the following subsection.

## B. Virtual Work of Fluctuations

For non-extremal flows the local force balance equation can be written in the form

$$\mathscr{D} = MD_t V - F \tag{10a}$$

where

$$F \equiv -\frac{1}{n}\nabla p - M\nabla\phi . \tag{10b}$$

For extremal flow, Equation (10) reduces to Equation (9) and $\tilde{\mathscr{D}} = 0$. $\mathscr{D}$ can be interpreted as the molar d'Alembert force, whose vanishing is one way to specify an equilibrium flow. $\mathscr{D}$ can also be regarded as a molar displacement force that arises when a virtual displacement carries a one-mole sample of fluid away from its normal trajectory in the equilibrium flow. If this flow is stable, then $\mathscr{D}$ will tend to restore the displaced sample to its original trajectory, and positive work will be required to produce the displacement. If $\delta A$ is the amount of work required to displace one mole of fluid a distance $\delta X$, and $\mathscr{D}(\delta X)$ is the displacement force at the end of the displacement, then $\mathscr{D}_{AV} = \frac{1}{2}\mathscr{D}(\delta X)$ is the average value of $\mathscr{D}$ during the displacement, and

$$\delta^{(2)}A = -\delta X \cdot \mathscr{D}_{AV} = -\tfrac{1}{2}\delta X \cdot \mathscr{D}(\delta X) . \tag{11}$$

This work is of second order in $(\delta X)$ because it is $\delta X$ itself that gives rise to $\mathscr{D}$. In the case of a displacement from a non-equilibrium flow (indicated by an overhead bar) for which $\bar{\mathscr{D}} \neq 0$, then the work is of first order in $\delta X$:

$$\delta^{(1)}A = -\delta X \cdot \bar{\mathscr{D}} = -\delta X \cdot (M\bar{D}_t\bar{V} - \bar{F}) \tag{12}$$

where use has been made of Equation (10a). If $\delta^{(1)}a$ is the corresponding work density involved in displacing the $\bar{n}$ moles that occupy unit volume then

$$\delta^{(1)}a = \bar{n}\delta^{(1)}A = \delta^{(1)}n \cdot (\bar{F} - M\bar{D}_t\bar{V}) \tag{13}$$

where $\delta^{(1)}n = \bar{n}\,\delta X$ is the first-order mole displacement flux defined in Equation (44) of Paper I. The natural second-order generalization of Equation (13) is

$$\delta^{(1+2)}a = \delta^{(1+2)}n \cdot (\bar{F} - M\bar{D}_t\bar{V}) = -\delta^{(1+2)}n \cdot \bar{\mathscr{D}} \tag{14}$$

where, to $O^2(\delta X)$, $\delta^{(1+2)}\mathbf{n}$ can be written in any of the following forms:

$$\delta^{(1+2)}\mathbf{n} = (\bar{n} + \tfrac{1}{2}\delta^{(1)}n)\,(\delta X + \tfrac{1}{2}\delta X \cdot \nabla \delta X) \tag{15a}$$

$$= (\bar{n} + \delta^{(1)}n)\,\delta X + \tfrac{1}{2}\nabla \cdot (\delta X \bar{n} \delta X) \tag{15b}$$

$$= \bar{n}(\delta X + \delta X \cdot \nabla \delta X) - \tfrac{1}{2}\nabla \cdot (\delta X \bar{n} \delta X) \tag{15c}$$

where

$$\delta^{(1)}n = -\nabla \cdot (\bar{n}\,\delta X) = -\nabla \cdot \delta^{(1)}\mathbf{n}\,. \tag{15d}$$

As noted in Equation (44) of Paper I, the first and second-order change in mole density is given by

$$\delta^{(1+2)}n = -\nabla \cdot \delta^{(1+2)}\mathbf{n}\,. \tag{16}$$

The displacement force $\mathscr{D}(\delta X)$ and the corresponding second-order work is calculated in the following subsection for a virtual displacement of a mole of fluid in a density-stratified atmosphere. These expressions will help clarify the physical implications implicit in the second variations presented in Sections IV and V, but the expressions for $\delta^{(2)}A$ derived below enter in no way into the derivations of Sections IV and V.

### C. Buoyancy Force and Work

If $\tilde{n}(\boldsymbol{x})$ is the equilibrium density at the fixed observation point $\boldsymbol{x}$, then if the matter is subjected to a displacement field $\delta X$, the matter at the point $\boldsymbol{x}$ after the displacement is that which had occupied the point $\boldsymbol{x} - \delta X$ before the displacement. If, moreover, the displacement is of the Boussinesq type, i.e. density-preserving, then the density $n'(\boldsymbol{x})$ observed at the point $\boldsymbol{x}$ after the displacement is $n' = \tilde{n} - \delta X \cdot \nabla \tilde{n} = \tilde{n}(1 - \delta X \cdot \nabla \ell n\, \tilde{n})$. If the velocity and acceleration fields are unchanged by the virtual displacement, and $\mathbf{F}'$ is the new force at $\boldsymbol{x}$ after the displacement, then $\mathscr{D}$ is defined by $\mathbf{F}' \equiv \tilde{\mathbf{F}} + \mathscr{D}$, so that it follows from Equation (10) that

$$\mathscr{D}(\delta X) = F' - \tilde{F} = -\frac{1}{n'}\nabla\tilde{p} + \frac{1}{\tilde{n}}\nabla\tilde{p}$$

$$= -(\delta X \cdot \nabla \ell n\, \tilde{n})\left(\frac{1}{\tilde{n}}\nabla\tilde{p}\right) + O^2(\delta X). \tag{17}$$

Using this in (11), it follows that

$$\delta^{(2)}A_B = +\frac{1}{2\tilde{n}}[(\nabla \ell n\, \tilde{n})(\nabla\tilde{p})]:(\delta X \delta X) + O^3(\delta X) \tag{18}$$

is the second-order work that must be performed in order to carry out a Boussinesq displacement $\delta X$ of one mole of fluid. Using

$$\nabla\tilde{p} = -\tilde{n}(M\nabla\tilde{\phi} + \tilde{F}) = -\tilde{n}M(\nabla\tilde{\phi} + \tilde{D}_t\tilde{V}) \tag{19}$$

to eliminate $\nabla\tilde{p}$ in (18) yields

$$\delta^{(2)}A_B = -\tfrac{1}{2}M[(\nabla \ell n\, \tilde{n})(\nabla\tilde{\phi} + \tilde{D}_t\tilde{V})]:(\delta X \delta X). \tag{20}$$

For $\tilde{D}_t\tilde{V} = 0$ one obtains the familiar expression for the work involved in a Boussinesq displacement of one mole of gas in a static atmosphere. If this work is positive, the atmosphere is stable. For $\nabla\tilde{\phi} = 0$, one obtains the corresponding expression that predicts the onset of Rayleigh–Taylor instability,[7] i.e. instability resulting from the acceleration of a stratified fluid in the direction of increasing density. The fact that $\nabla\tilde{\phi}$ and $\tilde{D}_t\tilde{V}$ enter into the stability criterion in the same way is in keeping with the Equivalence Principle.

The Boussinesq-type displacements may be visualized as occurring so fast that the displaced blob of gas does not have sufficient time to change its volume in response to the changing external pressure that it feels. The opposite idealization is the quasi-static displacement that occurs so slowly that at every point of its displacement trajectory the internal pressure of the blob is equal to the external ambient pressure. This gives rise to the Väisälä–Brunt stability criterion[8,9] which will be derived below. First, however, a more general expression will be derived that is appropriate to the case of a completely arbitrary

change in the volume of the blob during its displacement. This is done by taking into account the change in enthalpy of the blob that corresponds to an arbitrary adiabatic volume change. Since $(\partial H/\partial p)_S = \hat{V}$ and $(\partial^2 H/\partial p^2)_S = -\hat{V}/\beta$ where $\beta$ is the adiabatic bulk modulus defined by

$$\beta \equiv -\hat{V}\left(\frac{\partial p}{\partial \hat{V}}\right)_S = n\left(\frac{\partial p}{\partial n}\right)_S , \tag{21}$$

it follows that for a one-mole blob

$$\begin{aligned}(\delta^{(1+2)}H)_S &= \hat{V}(\delta p)_S - \tfrac{1}{2}\frac{\hat{V}}{\beta}(\delta p)_S^2 \\ &= -\beta\delta\hat{V} - \tfrac{1}{2}\frac{\beta}{\hat{V}}(\delta\hat{V})^2\end{aligned} \tag{22}$$

where use has been made of

$$(\delta p)_S = -\frac{\beta}{\hat{V}}\delta V \tag{23}$$

which follows from (21). An expression for $\delta\hat{V}$ in terms of $\delta X$ follows from the identity given in Equation (9a) of Paper I:

$$\delta\hat{V} = (\partial\hat{V}/\partial G_A)\cdot\delta G_A = \hat{V}G^A\cdot(\partial_A\delta X) = \hat{V}(\nabla\cdot\delta X) . \tag{24}$$

The first-order part of (22) is not of interest because it will generally average to zero over an extensive layer of fluid at a given geopotential height. Adding the second-order part of (22) to (18), one obtains the following expression for the net second-order energy $\delta^{(2)}A$ that must be supplied in order to carry out the displacement $\delta X$ of one mole of fluid that simultaneously undergoes an arbitrary adiabatic volume change $\delta\hat{V} = \hat{V}(\nabla\cdot\delta X)$:

$$\delta^{(2)}A = \frac{1}{2\tilde{n}}[(\delta X\cdot\nabla\ell n\,\tilde{n})(\delta X\cdot\nabla\tilde{p}) - \tilde{\beta}(\nabla\cdot\delta X)^2] . \tag{25}$$

The Väisälä-Brunt specialization of this expression results from requiring that the adiabatic internal pressure change $(\delta p)_S$ in (23) be equal to the external pressure change

$\delta \mathbf{X} \cdot \nabla \tilde{p}$. Combining this requirement with (24), one finds that

$$\nabla \cdot \delta \mathbf{X} = -\delta \mathbf{X} \cdot \nabla \tilde{p}/\tilde{\beta} \quad (\text{if } \delta p_{INT} = \delta p_{EXT}) \tag{26}$$

is the condition that must be satisfied in order that the internal and external pressures remain in equilibrium. The expression for the second-order Väisälä-Brunt work of displacement $\delta^{(2)} A_{VB}$ results upon substitution of (26) into (25):

$$\delta^{(2)} A_{VB} = \frac{1}{2\tilde{n}} [(\delta \mathbf{X} \cdot \nabla \ell n \tilde{n}) - \frac{1}{\tilde{\beta}} (\delta \mathbf{X} \cdot \nabla \tilde{p})] (\delta \mathbf{X} \cdot \nabla \tilde{p}) . \tag{27}$$

For the case of a flat static atmosphere for which $\delta \mathbf{X} \cdot \nabla \tilde{p} = -\tilde{n} M g \delta Z$ where $g$ is the acceleration of gravity, and $\tilde{\beta} = \tilde{n} M \tilde{C}^2$ is used to eliminate $\tilde{\beta}$ in favor of the speed of sound $\tilde{C}$, (27) becomes

$$\delta^{(2)} A_{VB} = -\tfrac{1}{2} M g \left( \frac{d \ell n \tilde{n}}{dz} + \frac{g}{\tilde{C}^2} \right) (\delta Z)^2 . \quad (\text{flat, static atmosphere}) \tag{28}$$

The expression (27) can be simplified somewhat by making use of the thermodynamic identity

$$d \ell n \, n - \frac{1}{\beta} dp = - \frac{\alpha T}{Cp} dS = -\left( \frac{\gamma - 1}{\alpha T} \right) \frac{n}{\beta} T dS \tag{29}$$

where

$$\gamma \equiv \frac{C_p}{C_V} = \frac{(\partial S/\partial T)_p}{(\partial S/\partial T)_V} \tag{30}$$

is the ratio of specific heats and

$$\alpha \equiv \frac{1}{\hat{V}} \left( \frac{\partial \hat{V}}{\partial T} \right)_p = -\left( \frac{\partial \ell n \, n}{\partial T} \right)_p \tag{31}$$

is the coefficient of thermal expansion. Using (29) in (27), one obtains

$$\delta^{(2)} A_{VB} = -\frac{1}{2\tilde{\beta}} \left( \frac{\widetilde{\gamma - 1}}{\alpha T} \right) [(\tilde{T} \nabla \tilde{S}) (\nabla \tilde{p})] : (\delta \mathbf{X} \delta \mathbf{X}) . \tag{32}$$

**D. Dual Aspects of Pressure**

The pressure $p(\hat{V}, S)$ defined by Equation (5), or $p(n, S)$ defined by Equation (8), has the dimensions of energy density, a fact that is immediately evident both from the definitions as well as from the relation $p = h - u$ where $h \equiv nH$ is the enthalpy density. On the other hand, the appearance of $(-p)$ in Equation (6) as the thermodynamic conjugate of $\hat{V}$ indicates that pressure should be regarded as an **intensive** quantity. The importance of this duality in the description of fluctuations away from thermodynamic equilibrium will be explained in Section III. Suffice it to say at this point that, in the case of a turbulent gas in which fluctuations about the equilibrium density $\tilde{n}$ are occurring, p as defined by Equation (5) or Equation (8) is to be regarded as the instantaneous pressure **within** a sample of gas that is so small that the changes induced by its fluctuating volume may be regarded as quasi-static, so the use of the **equilibrium** state function $U(S, \hat{V})$ (or $u(S, n)$) is justified. The **intensive pressure** (which will be designated by P), on the other hand, is insensitive to the fluctuating density changes, and is to be regarded as describing the local **average** pressure, the average being taken over a sufficiently large space-time interval so that the effects of the fluctuating density vanish. Thus P represents the average pressure existing **outside** of any given small fluctuating sample, and will be called the **external pressure**, whereas p will be called the **internal pressure**.

In the more complete treatment[6] alluded to following Equation (8), the intensive pressure $P = P(G, T)$ was represented as a function of temperature and of molar Gibbs function G (or, in the case of several interacting chemical constituents or phases, of the appropriate partial molar Gibbs function or chemical potential). In the truncated, but simpler, treatment that will be developed in this paper, the intensive or external pressure P will be represented as a function of the molar enthalpy H and of the molar entropy S. Because $S = S(\Lambda, t)$ is specified at the outset, one of the two thermodynamic degrees of

freedom is effectively suppressed in the truncated formalism. The function $P = P(H, S)$ is a canonical state function from which all other thermodynamic quantities can be derived by differentiation. The mole density $N(H, S)$ and the temperature $T(H, S)$ are given by

$$dP = NdH - NTdS . \tag{33}$$

The "external mole density" N must be distinguished from the "internal mole density" n, except at equilibrium when the two are equal:

$$N(\tilde{H}, \tilde{S}) \equiv \tilde{N} = \tilde{n} \equiv J_x^{\tilde{\Lambda}}. \tag{34}$$

(In principle, different symbols should be used for $T(H, S)$ defined by Equation (33) and $T(S, \hat{V})$ defined by Equation (6), but, because $S = S(\Lambda, t)$ is specified, it turns out that the need for this distinction does not arise.) Corresponding to the interpretation of P, N can be interpreted as the average mole density in the fluid surrounding a small sample whose internal mole density n is rapidly fluctuating.

The dual pressure functions p and P can be used to generate dual internal energy functions U and $\mathcal{U}$ and the corresponding energy densities $u$ and $\mathcal{u}$. These quantities satisfy important inequalities, which will now be derived. It is easily shown that the adiabatic second variation of $u(S, n)$ is $(\delta^{(2)}u)_S = \tfrac{1}{2}(\tilde{\beta}/\tilde{n}^2)\,(\delta n)^2 \geqslant 0$ where the equality corresponds to $\delta n = 0$. To $O^3(\delta n)$ this second variation can also be represented as the difference between $(u - \tilde{u})$ and $(\delta^{(1)}u)_S$ where it follows from Equation (7) that $(\delta^{(1)}u)_S = \tilde{H}\delta n = \tilde{H}(n - \tilde{n})$. Thus the following inequality is valid:

$$(u - \tilde{u}) - \tilde{H}(n - \tilde{n}) \geqslant 0 \tag{35}$$

where the equality holds only if $n = \tilde{n}$. (It should be noted that this inequality is valid only if both $u$ and $\tilde{u}$ correspond to $\tilde{S}$, i.e. only n may vary. In the more general treatment[6] based on $u(\mathcal{s}, n)$ rather than $u(S, n)$, an inequality can be derived in which both $\mathcal{s}$ and n are free to vary.) Using the fact that $\tilde{H}\tilde{n} - \tilde{u} = \tilde{p} = \tilde{P}$, Equation (35) can be written in the following form:

$$u(n, \tilde{S}) - \mathcal{u}(n, \tilde{H}, \tilde{S}) \geqslant 0 \tag{36}$$

where

$$\begin{aligned} \mathcal{U}(n, \tilde{H}, \tilde{S}) &\equiv n\tilde{H} - P(\tilde{H}, \tilde{S}) \\ &= n\mathcal{U}(\tilde{H}, \hat{V}, \tilde{S}) \end{aligned} \tag{37}$$

where

$$\mathcal{U}(\tilde{H}, \hat{V}, \tilde{S}) \equiv \tilde{H} - \hat{V}P(\tilde{H}, \tilde{S}) . \tag{38}$$

Because $u(n, \tilde{S}) = nU(\hat{V}, \tilde{S})$, Equation (36) can also be written

$$U(\hat{V}, \tilde{S}) - \mathcal{U}(\tilde{H}, \hat{V}, \tilde{S}) \geqslant 0 . \tag{39}$$

The equality holds only when the redundant set of three variables $(\tilde{H}, \hat{V}, \tilde{S})$ is consistent with the relation $H = U - \hat{V}(\partial U/\partial \hat{V})_S$. Because the equilibrium point involved in Equations (36) and (39) is arbitrary, the tilde can be omitted from $\tilde{H}$ and $\tilde{S}$. The inequality itself will then determine the equilibrium point, namely that set of values for which the equality holds.

The physical significance of these inequalities and their relation to the Second Law of Thermodynamics will be explained in Section III. The importance of a similar inequality (in the entropy representation rather than the energy representation used here) in non-equilibrium thermodynamics has been emphasized by Tisza.[10] The generalization of the above inequalities that refers to a stratified atmosphere in a gravitational field will be given in Section V.

If the pressure that appears in Euler's equation given in Equation (9) is represented by P(H, S) rather than by p(n, S), an extra equation of motion is necessary to guarantee the consistency of these two representations. The obvious choice is just $\tilde{P} = \tilde{p}$, but it will be shown in Section V that it is the equivalent requirement $\tilde{N} = \tilde{n}$ given in Equation (34) that falls out of the variational analysis.

In the variational analysis, the functional form of $H(\Lambda, t)$ is not known in advance. It must be specified by the variational principle. If $\tilde{H}(\Lambda, t)$ is the functional dependence that is consistent with $\tilde{P} \equiv \tilde{p}$ or $\tilde{N} = \tilde{n}$, then for a slightly different functional dependence $H(\Lambda, t) = \tilde{H}(\Lambda, t) + \epsilon(\Lambda, t)$ where $\epsilon$ represents the variation in H. In the convected frame in which $(\Lambda^A, t)$ are the independent variables, this is the only variation that has to be taken into account. In an inertial-frame analysis, however, each of the functions $\tilde{H}(\Lambda, t)$ and $\epsilon(\Lambda, t)$ has a variation of the form given by Equation (4) that results from the variation of the functional forms of $\Lambda^A(\boldsymbol{x}, t)$. Thus, taking into account that $\dot{\epsilon}$ is already of first-order magnitude, the total variation of $H(\Lambda, t)$ in an inertial frame analysis is

$$\begin{aligned} \delta^{(1+2)}H = {} & -\delta X \cdot \nabla\tilde{H} + \tfrac{1}{2}(\delta X \delta X : \nabla\nabla\tilde{H}) \\ & + \epsilon(\tilde{\Lambda}, t) - \delta X \cdot \nabla\epsilon(\tilde{\Lambda}, t) . \end{aligned} \tag{40}$$

An expression of this form is also valid for the variation about a non-extremal functional dependence $\bar{H}[\bar{\Lambda}(\boldsymbol{x}, t); t]$. In Sections V and VI the functional variation $\epsilon(\bar{\Lambda}, t)$ will be designated by $\delta_H H$ to indicate that it is the first-order variation resulting from the variation in the functional dependence of $H(\Lambda, t)$ on $\Lambda^A$ and t.

## E. Entropy Fluctuations

The use of $p(\hat{V}, S)$ or $p(n, S)$ to describe the pressure implies that equilibrium thermodynamics is valid for non-extremal trial functions as well as for the extremal configuration. That is, the fluctuations about the extremum are effectively quasi-static. This is consistent with the interpretation of the prescribed function $S(\Lambda, t)$ as the instantaneous molar entropy which, except for the prescribed time-dependence, is a constant of motion even during the fluctuations.

The use of $P(H, S)$, however, involves a redundancy that implies that equilibrium thermodynamics is valid only for the extremal set of trial functions (or, more exactly, for

any set of trial functions for which Equation (34) holds). In this case, $S(\Lambda, t)$ can no longer be interpreted as the instantaneous molar entropy. Rather, it must be regarded as the prescribed time-average of the entropy about which the instantaneous entropy fluctuates. Only for trial functions for which Equation (34) is satisfied is the instantaneous molar entropy equal to $S(\Lambda, t)$. In the convected frame, this average entropy $S(\Lambda, t)$ does not fluctuate at all. It is, however, possible to define the **instantaneous** entropy fluctuation $\delta S$ by means of the following familiar relation:

$$\delta Q \equiv T\delta S = \delta H - \delta P/n . \tag{41}$$

If $\delta Q$ is used rather than $T\delta S$, this relation is merely a statement of the First Law in which $\delta Q$ is the heat energy absorbed by the sample of fluid from its surroundings. In general $\delta P$ depends on $\delta X$ as well as on $\delta H$, so $\delta P$ and $\delta H$ are independent. Two special cases will be of interest in what follows:

$$\delta_H Q \equiv \delta_H H - \delta_H P/n = \left(1 - \frac{N}{n}\right) \delta_H H \tag{42a}$$

and

$$\delta_X Q \equiv \delta_H H - (\delta X \cdot \nabla P)/n \tag{42b}$$

where in Equation (42a)

$$\delta_H P \equiv (\partial P/\partial H)_S \, \delta_H H = N\delta_H H \tag{42c}$$

is the external pressure change produced by $\delta_H H$. The $\delta_H Q$ of Equation (42a) represents the increase in molar heat produced by the random "sloshing about" of enthalpy in the fluid. The $\delta_X Q$ in Equation (42b) is the change in heat that corresponds to departure from isentropy during the displacement of a fluid blob in a pressure gradient. For example, if the upward quasi-static displacement of a blob in a stratified atmosphere is isentropic, then $\delta_X Q = 0$. If $\delta_X Q \neq 0$, this could mean either that heat has been exchanged between the blob and its surroundings, or that there has been a spontaneous conversion of internal thermal energy into ordered form.

In the entropy representation, a stable equilibrium of an isolated system is characterized by a maximum value of the total entropy S,[11] i.e. $\delta^{(1)}S = 0$, $\delta^{(2)}S \leqslant 0$ where the $\delta$ indicates a virtual fluctuation from equilibrium. (The inequality is reversed for a real spontaneous change.) If the system is immersed in a heat reservoir, then $\delta^{(1)}S \neq 0$, but it is still necessary that $\delta^{(2)}S \leqslant 0$ since otherwise a virtual fluctuation that exchanged heat with the reservoir could produce a second-order increase in the total entropy of the system plus reservoir which would contradict the posited stability of the system and its reservoir.

In the energy representation used here the corresponding statements can be made about the total change in internal heat $\delta Q$. The second-order change $\delta^{(2)}Q$, which cannot be accounted for by simple heat exchange with the reservoir, can be interpreted as the change in the **unavailable energy** of the system. The requirement $\delta^{(2)}Q \leqslant 0$ for virtual fluctuations in a stable system is equivalent to the statement that the unavailable energy of a stable system and its reservoir is a maximum. Thus virtual fluctuations correspond to conversions of internal thermal energy into some ordered form of energy, i.e. virtual fluctuations convert unavailable energy into available form.

An alternative interpretation of the condition $\delta^{(2)}Q$ results from the following argument:

$$\begin{aligned}\delta^{(1+2)}Q &= \int_N \delta Q d^3(\Lambda) = \int_V \delta Q n d^3(x) = \int_V (\tilde{n} + \delta^{(1)}n)\delta Q d^3(x) \\ &= \int_V \tilde{n}\delta Q d^3(x) + \int_V \delta^{(1)}n\,\delta Q d^3(x)\,.\end{aligned} \tag{43}$$

The first integral is the first-order change in total internal heat which vanishes if the system is isolated or else cancels with the heat absorbed by the reservoir, if the system is not

isolated. The second-order integral depends on the integrated correlation between $\delta^{(1)}n$ and $\delta Q$, and is completely independent of any heat change of the reservoir. Thus a necessary condition for stability is

$$\delta^{(2)}Q = \int_V \delta^{(1)}n\, \delta Q d^3(x) \leqslant 0 . \tag{44}$$

This condition has a very simple interpretation. It requires that, on the average, a positive value of $\delta Q$ must be accompanied by a negative value of $\delta^{(1)}n$ and vice versa. This means that, on the average, when heat flows into a sample of fluid from the surroundings, the sample must expand, and must contract when heat leaves. This eminently reasonable condition is not automatically satisfied by the fluctuations in the trial functions of Sections V and VII. Thus it represents a constraint that in principle must either be imposed on the parameterization of the trial functions, or on the procedures involved in a direct numerical solution. It is, however, a very weak constraint whose violation does not produce spurious answers, but rather only introduces the possibility of numerical instabilities into the solution process. This point is further discussed in Section VII F.

It should be noted that "virtual" fluctuations are virtual in the sense that they (locally) violate the Second Law. This does not imply that they cannot happen in nature. The Second Law refers only to a macroscopic sample of fluid, and not to fluctuations at the microscopic level. It is necessary, however, that whatever correlations exist between fluctuations at different points be such that at a macroscopic level no Second-Law violations occur. This is the meaning of the condition in Equation (44). Because physical fluctuations are never instantaneous, the integral involved in this condition should really extend over time as well as space. Such a space-time integral is actually what results from a calculation of the second variations of the variational principle discussed in Sections V and VII.

## F. Internal Free Energy

The $\delta A \equiv -\delta X \cdot \mathscr{D}$ that was introduced in subsection B above is the molar deformation work, that is, the work done against the molar deformation force $\mathscr{D}$ defined in Equation (10a). The integral of this over the entire fluid, $\delta A \equiv \int \delta A\, dN$, represents the amount of energy that has been stored in the fluid by virtue of carrying out the deformation associated with the displacement field $\delta X$. Inasmuch as this energy could in principle be extracted again from the fluid, it represents a potential energy and, if $\delta A$ were in fact a total differential, A could be called the "deformation potential." However, it is not justified to assume that $\delta A$ is a total differential. In fact, when entropy fluctuations are taken into account, the integral of $-\delta X \cdot \mathscr{D}$ no longer represents the amount of useful energy that could in principle be extracted from the fluid by relaxing the deformation displacements. The reason for this is that if the displacements $\delta X$ are accompanied by an entropy increase $\delta S$, then a part $\delta Q \equiv T\delta S$ of the molar work of deformation is degraded and becomes unavailable for conversion into useful form. The $\delta A$ discussed in subsections B and C above should properly be designated $(\delta A)_S$ to indicate that all of the displacements were isentropic. This followed automatically from the fact that the pressure was represented by $p(\hat{V}, S)$. With the introduction of the extra degree of freedom involved in the P(H, S) representation, the $\delta Q$ defined by Equation (41) must be included in the formalism. Thus if $\delta A$ represents the convertible or "free" part of the deformation energy,

$$\delta A = (\delta A)_S - \delta Q \tag{45a}$$

$$= (-\delta X \cdot \mathscr{D}) - (\delta H - \delta P/n)\,. \tag{45b}$$

It was pointed out in Equation (12) that $\delta A$ is of first order if $\bar{\mathscr{D}} \neq \tilde{\mathscr{D}} = 0$ has a finite value that is independent of $\delta X$. Correspondingly, $\delta Q$ is of first order if $\bar{N} \neq \bar{n}$ and has the value given in (42a). Thus the generalization of Equation (12) is

$$\delta^{(1)}A = -\delta X \cdot \mathscr{D} - (1 - \bar{N}/\bar{n})\,\delta_H H\,. \tag{46}$$

If H is a primitive function in the variational analysis, i.e. if $H(\Lambda, t)$ is one of the trial functions, then $\delta_H H = \delta_H^{(1)} H$ has no second-order variation. If, however, H is expressed as a function of other functions which are regarded as primitive, then $\delta_H H$ can have a second-order dependence. For example, if H is represented as the Jacobian $H \equiv J_\Lambda^\eta \equiv \det(\partial\eta^A/\partial\Lambda^B)$ where the three functions $\eta^A(\Lambda, t)$ are regarded as primitive, then $\delta H = \det(\partial\delta\eta^A/\partial\Lambda^B)$ is of third order in $\delta\eta^A$. Allowing for the possibility of some such representation of H, the generalization of Equation (14) becomes

$$\delta^{(1+2)}a = -\delta^{(1+2)}n \cdot \bar{\mathscr{D}} - \bar{n}\delta_H^{(1+2)}Q \tag{47a}$$

$$= \delta^{(1+2)}n \cdot (\bar{F} - M\bar{D}_t\bar{V}) + (\bar{N} - \bar{n})\,\delta_H^{(1+2)}H \tag{47b}$$

where $\delta^{(1+2)}a$ is the free deformation energy density.

At equilibrium, $\tilde{N} = \tilde{n}$ and so $\delta_H Q = 0$ even if $\delta_H H \neq 0$. In this case, however, it is possible for correlations to exist between $\delta_H H$ and $\delta X$ such that $\delta^{(2)}Q \neq 0$. In fact, the correlations are just those between $\delta Q$ and $\delta^{(1)}n = -\nabla \cdot (\tilde{n}\delta X)$ that were discussed following Equation (44). For the displacement of a one-mole blob of fluid through a pressure gradient the appropriate $\delta Q$ is the $\delta_X Q$ given in Equation (42b). The appropriate $(\delta A)_S$ to use in the neighborhood of equilibrium for which $\tilde{\mathscr{D}} = 0$ is the second-order expression given in Equation (11). If this is augmented by the work of adiabatic expansion given in Equation (22), the expression for $(\delta^{(2)}A)_S$ given in Equation (25) results. Combining this with Equation (42b), it follows that in the neighborhood of equilibrium

$$\delta^{(2)}A = \int_V \tilde{n}\left\{[-\tfrac{1}{2}\delta X \cdot \mathscr{D}(\delta X)]_S + [\delta_X^{(2)}H]_S\right\} d^3(x) - \delta^{(2)}Q \tag{48a}$$

$$= \int_V \tfrac{1}{2}[(\delta X \cdot \nabla \ell n\, \tilde{n})(\delta X \cdot \nabla\tilde{p}) - \tilde{\beta}(\nabla \cdot \delta X)^2]\, d^3(x)$$

$$- \int_V (\delta^{(1)}n)(\delta_H H - \delta X \cdot \nabla\tilde{p}/\tilde{n})\, d^3(x)\,. \tag{48b}$$

The expressions in Equations (47b) and (48b) will be encountered again in Section V where they will result from a derivation that is entirely independent of any of the results derived above.

The $\delta A$ discussed above represents the free (i.e. convertible) part of the energy associated with the internal deformation of the system. For the sake of brevity, it will be called the variation of the **internal free energy** of the system. It will be shown in Section V that $\delta A$ can indeed be represented as a total differential, i.e. as the variation of a spatial integral over a specified functional. In this sense it is legitimate then to refer to A itself as the **total internal free energy** of the system. It should be emphasized that the use of the term "free energy" does **not** imply that A is to be identified with the familiar free internal energy (Helmholtz function) or the free enthalpy (Gibbs function). These functions refer to **equilibrium states** whereas A represents the convertible energy of **non-equilibrium** states. The numerical value of $\widetilde{A}$ for equilibrium is of little interest, because this can be arbitrarily changed without changing the variational properties of A. This corresponds to the fact that in classical mechanics the absolute value of any energy never has physical significance. Only differences or changes of energy are observable.

## G. Thermodynamic State Functions

It will be seen in Sections IV and V that the construction of an explicit functional for the total energy in the convected frame involves a knowledge of the functional form of $U(\hat{V}, S)$, the canonical state function for molar internal energy. The corresponding construction in an inertial frame involves knowing the functional form of $u(n, S)$. The construction of the functional for the free energy in either the convected frame or an inertial frame involves knowing the functional form of $P(H, S)$. Very often these state functions will either be known, or else can easily be constructed from empirically determined

thermodynamic functions. For example, for a perfect gas the three necessary functions have the following forms:

$$U(\hat{V}, S) = U_0(\hat{V}/\hat{V}_0)^{-(\gamma - 1)} \exp[(\gamma - 1)(S - S_0)/R] \; ; \tag{49}$$

$$u(n, S) = u_0(n/n_0)^{\gamma} \exp[(\gamma - 1)(S - S_0)/R] \; ; \tag{50}$$

$$P(H, S) = p_0(H/H_0)^{\gamma/(\gamma - 1)} \exp[-(S - S_0)/R] \; ; \tag{51}$$

where R is the molar gas constant and $U_0$, $\hat{V}_0$, $S_0$ etc. are reference values which may be either constants or else specified functions of ($\mathfrak{x}$, t) or of ($\Lambda^A$, t).

An alternative to using a known empirical state function is to construct a state function from the expressions for the first and second differentials of $U(\hat{V}, S)$, $u(n, S)$, or $P(H, S)$. The first differentials of these functions are given in Equations (6), (7), and (33) respectively. It is well known[12] that the second differential of a canonical state function for a simple fluid can be expressed in terms of an appropriately chosen set of three thermodynamic coefficients. The three coefficients used in the expressions below are the ratio of specific heats $\gamma$, the adiabatic bulk modulus $\beta$, and the coefficient of thermal expansion $\alpha$. The definitions of these quantities have been given in Equations (30), (21), and (31) respectively. For a perfect gas, $\gamma$ is a constant, $\beta = \gamma p$, and $\alpha = 1/T$. For an arbitrary fluid, $\beta$ can always be replaced by the speed of sound C by means of the relation $\beta = nMC^2$, which for a perfect gas becomes $\beta = n\gamma RT$. The intuitive significance of the dimensionless product $\alpha T$ can be seen from the relation $dH = C_p dT + (1 - \alpha T)\hat{V}dp$ which shows that the magnitude of $(1 - \alpha T)$ is a measure of the departure of the fluid from the perfect-gas relation $dH = C_p dT$. The necessary expressions for the second differentials of an arbitrary fluid are

$$\delta^{(2)}U(\hat{V}, S) = \tfrac{1}{2}n\beta(\delta\hat{V})^2 + \tfrac{1}{2}\frac{n\gamma(\gamma - 1)}{\alpha^2\beta}(\delta S)^2 - \frac{n(\gamma - 1)}{\alpha}\delta\hat{V}\delta S \; ; \tag{52}$$

$$\delta^{(2)}u(n, S) = \tfrac{1}{2}\frac{\beta}{n^2}(\delta n)^2 + \tfrac{1}{2}\frac{n^2\gamma(\gamma - 1)}{\alpha^2\beta}(\delta S)^2 + T\left(1 + \frac{\gamma - 1}{\alpha T}\right)\delta n\delta S \; ; \tag{53}$$

$$\delta^{(2)}P(H, S) = \tfrac{1}{2}\frac{n^2}{\beta}(\delta H)^2 + \tfrac{1}{2}\frac{n^2}{\alpha^2\beta}[(1 - \alpha T)^2 + \gamma(2\alpha T - 1)](\delta S)^2$$
$$- \frac{n^2 T}{\beta}\left(1 + \frac{\gamma - 1}{\alpha T}\right)\delta H \delta S . \tag{54}$$

These are the expressions that are used in Sections IV and V to calculate the second variations of the thermodynamic functions. This is done by substituting into the above expressions the already given expressions for $\delta\hat{V}$, $\delta n$, $\delta S$, and $\delta H$ in terms of $\delta\Lambda^A$ or $\delta\tilde{X}$ and $\delta_H H$.

Using Equations (52–54) and the corresponding first-order relations given in Equations (6), (7), and (33), the following expressions for the necessary canonical state functions can be constructed:

$$U(\hat{V}, S) = U_o - p_o(\hat{V} - \hat{V}_o) + T_o(S - S_o)$$
$$+ \tfrac{1}{2}(n\beta)_o\left[(\hat{V} - \hat{V}_o) - \left(\frac{\gamma - 1}{\alpha\beta}\right)_o (S - S_o)\right]^2 \tag{55}$$
$$+ \tfrac{1}{2}\left[\frac{n(\gamma - 1)}{\alpha^2\beta}\right]_o (S - S_o)^2 ;$$

$$u(n, S) = u_o + H_o(n - n_o) + (nT)_o (S - S_o)$$
$$+ \tfrac{1}{2}\left(\frac{\beta}{n^2}\right)_o\left[(n - n_o) + \left(\frac{n^2 T}{\beta}\right)_o \left(1 + \frac{\gamma - 1}{\alpha T}\right)_o (S - S_o)\right]^2 \tag{56}$$
$$- \tfrac{1}{2}\frac{(nT)_o^2}{\beta_o}\left[1 + \left(\frac{\gamma - 1}{\alpha T}\right)_o \left(2 - \frac{1}{\alpha T}\right)_o\right](S - S_o)^2 ;$$

$$P(H, S) = p_o + n_o(H - H_o) - (nT)_o (S - S_o)$$
$$+ \tfrac{1}{2}\left(\frac{n^2}{\beta}\right)_o [(H - H_o) - T_o\left(1 + \frac{\gamma - 1}{\alpha T}\right)_o (S - S_o)]^2 \tag{57}$$
$$- \tfrac{1}{2}\left[\frac{n^2\gamma(\gamma - 1)}{\alpha^2\beta}\right]_o (S - S_o)^2 .$$

As in Equations (49–51), the coefficients and reference quantities are indicated by subscript o, and may either be constants, or consistently specified functions of either ($\boldsymbol{x}$,t) or ($\Lambda^A$, t).

The second-order parts of Equations (55–57) have been written in a form that makes the convexity properties explicit. In all three cases, if $S - S_o = 0$, the second-order parts are positive-definite, but if $S - S_o \neq 0$, this is true only in the case of $U(\hat{V}, S)$. The indefiniteness of the convexity of $u$(n, S) and P(H, S) is a consequence of the simplification that resulted from basing the thermodynamic formalism on these functions instead of using the functions $u$(n, $\delta$) and P(G, T) that were referred to following Equations (8) and (35) and at the beginning of Section II D. It will be seen in Sections IV and V, however, that the lack of definiteness of the convexity of $u$(n, s) and P(H, S) does not manifest itself in the convexity properties of the integral functionals in whose integrands they appear. That this should be the case is already apparent from the fact that, since S like $S_o$ must be a specified function of ($\Lambda^A$, t), if the coefficients and reference quantities in Equations (56) and (57) are specified as functions of ($\Lambda^A$, t), then $S_o$ can be specified so that $S - S_o = 0$, in which case the second-order parts of $u$(n, S) and P(H, S) are positive-definite functions of $(n - n_o)^2$ and $(H - H_o)^2$. This procedure simply puts the entropy dependence into the quantities $u_o$, $H_o$, $n_o$ and $\beta_o$, and the remaining dependence on $\delta n$ or $\delta H$ is positive-definite in second order.

As a practical matter, however, there exist many meteorological problems in which it would be preferable to specify the reference quantities in terms of ($\boldsymbol{x}$, t) in spite of the added complication that arises from the need to retain the terms involving $S - S_o$. For example, in the case of a direct variational solution of a closed convection cell embedded in a given static atmosphere, if the reference quantities were chosen to be the functions of

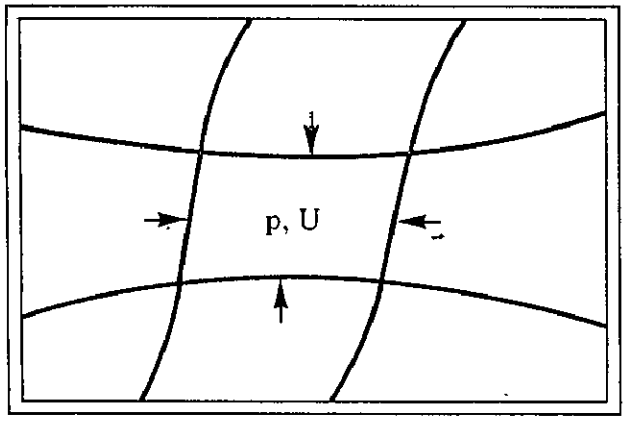
($\mathcal{X}$, t) appropriate to the static atmosphere, then the thermodynamic aspects of the variational problem would involve only small deviations from the given static atmosphere.

## III. DUAL PRINCIPLES OF VIRTUAL WORK

The dual pressure functions, $p(\hat{V}, S)$ and $P(H, S)$, and the dual energy functions, $U(\hat{V}, S)$ and $\mathcal{U}(H, \hat{V}, S)$, that were introduced in Section II D, correspond to the two different ways that the Principle of Virtual Work can be adapted to a continuum. These are illustrated in Figure 1 for the case of a homogeneous box of gas in the absence of a gravitational field.

Figure 1A illustrates the form of the principle in which the virtual work that is to be associated with a small cell that contains one mole of fluid is performed by an **external energy source** that acts against the **internal pressure** p of the cell, thereby increasing the internal energy of the cell by the amount $\delta_V U = -p\delta\hat{V}$. Figure 1B illustrates the form of the principle in which the gas within the cell in question spontaneously converts some of its internal energy into work of expansion against the surrounding external pressure P. This form of the principle involves an **internal energy source** (the gas itself) acting against the **external pressure** P. The work performed by the cell on its surroundings is $\delta_V A = +P\delta\hat{V}$. Referring to Equation (38), it is evident that $\delta_V \mathcal{U} \equiv (\partial\mathcal{U}/\partial\hat{V})_{H,S}\delta\hat{V} = -P(H,S)\delta\hat{V}$. Thus it follows that $\delta_V A = -\delta_V \mathcal{U}$. This just says that the work performed on the fluid surrounding the cell in question (i.e. the energy increase in the surrounding fluid) is bought at the expense of the thermal energy of the gas within the cell. Thus thermal energy within the cell has been spontaneously converted into ordered compressive energy residing in the surrounding fluid. Although such spontaneous conversion would be a violation of the Second Law on a macroscopic scale, it does happen on a microscopic scale. Thus the form of the Principle of Virtual Work that is illustrated in Figure 1B constitutes a rudimentary representation of the energetics of spontaneous fluctuation about equilibrium in a stable fluid. (Such fluctuation will be called "virtual" in order to distinguish it from real irreversible changes in a fluid that carry it from one equilibrium state to another.)

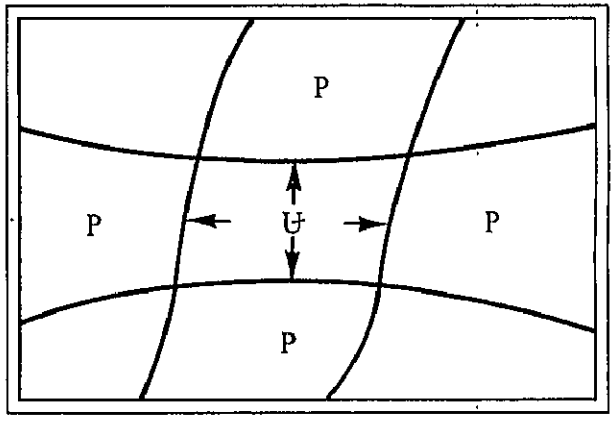
(A)




$\delta_V U = -p\delta\hat{V}$

DIRICHLET PRINCIPLE

(B)




$\delta_V U = -P\delta\hat{V}$

CASTIGLIANO PRINCIPLE

Figure 1. Virtual Work Performed on a Box of Gas in Deforming its Lagrange Surfaces. (A) Work Performed by an External Energy Source that Produces a Quasi-Static Deformation Against the Inter Pressure p. (B) Work Performed by Spontaneous Conversion of Thermal Energy Within a Small Sample of Gas into Work of Expansion Against the Surrounding Pressure P.

Whereas the form of the Principle of Virtual Work that involves P and $\mathcal{U}$ corresponds to the fluctuations that actually occur in a turbulent fluid, the form of the principle pictured in Figure 1A that involves p and U describes a purely imaginary kind of fluctuation that requires the intervention of an external agent that must not only provide energy, but must also provide internal barriers of some kind against the pressure differences that develop in the fluid as a result of the density changes produced by the fluctuations. The reason for this is that the use of the equilibrium state function $U(\hat{V}, S)$, and the corresponding equilibrium pressure $p \equiv -\partial U/\partial \hat{V}$, implies that the fluctuations are quasi-static. Thus inertial forces cannot be invoked in order to account for the difference between the internal pressure of a sample and the pressure of its external surroundings. (Such inertial forces can be invoked in the case of Figure 1B, because equilibrium thermodynamics does not apply so the fluctuations are fast, rather than quasi-static.)

When the two different forms of the principle are used to determine stability properties, they can be characterized as First-Law and Second-Law criteria in the following sense: In the case of Figure 1A, because the fluctuations are quasi-static, the total entropy of the system remains constant, but the total energy does not. If all possible fluctuations about a given state of the system increase the total energy, then the state must be stable, because if the system is isolated there is no available source for the energy that would be necessary to change it. This is a **First-Law stability criterion.**

In the case of the spontaneous fluctuations represented by Figure 1B, the total energy is a constant. The total entropy, however, is not constant because the fluctuations involve the spontaneous conversion of thermal energy into ordered form. The change in $\mathcal{U}$ for the entire system is a measure of this conversion. If $\delta\mathcal{U} < 0$ for all possible fluctuations, this means that every conceivable change in the system involves a conversion of the thermal

energy $\mathcal{U}$ into ordered compressive energy. But this is a violation of the Second Law, so it cannot occur (except for microscopic "virtual" fluctuations that cannot grow to macroscopically observable size). Thus the state is stable by virtue of the **Second Law**.

The existence of dual forms of the Principle of Virtual Work has long been recognized in the context of the theory of static elastic structures, but both forms of the principle were stated in a way that involved only ordered energy, so the connection with the Second Law was never brought to light. The First-Law form of the principle that is based on the equilibrium expression for energy (Fig. 1A) is known in the elasticity literature as Dirichlet's Principle.[3, 13] The form of the principle that expresses the energy in terms of an **intensive** quantity (P in the case of a gas, stress in case of an elastic structure) rather than an **extensive** quantity ($\hat{\mathcal{V}}$ in the case of the gas, strain in the elastic case) is known as Castigliano's Principle[3, 14] (although it had earlier been enunciated by Ménabréa[15]). In the classical form of Castigliano's principle the energy source that produced the deformations of the system was pictured as an arrangement of ropes, pulleys, and weights, so it was just as imaginary as the energy source involved in Dirichlet's Principle. Because the ultimate energy source for the deformations in Castigliano's Principle was gravitational (hanging weights) a **deformation potential function** existed, and the principle consisted of the statement that stable equilibrium is characterized by a minimum value of the deformation potential. In the present development, the concept of "deformation potential" is replaced by that of "total internal free energy" of the system. The existence of such a quantity in integrated form, rather than as a (possibly imperfect) differential, cannot be assumed in advance. In Sections V and VII it is proved that such an integrated free energy does in fact exist for both static and moving fluid systems. The fluid generalization of Castigliano's Principle is the statement that the total internal free energy of the system is a (local) minimum for stable flow.

Because $\delta_V \mathcal{U} = -\delta_V A$, the change in $\mathcal{U}$ is the mirror image of the change in internal free-energy A, and the same is true of the integrated quantities $\mathcal{U}$ and A. Thus if A is minimum for a stable static atmosphere, then $\mathcal{U}$ must be maximum. In fact, since in classical mechanics only changes or differences in energies are observable, an arbitrary constant can be added to A, and this can be chosen so that $A = -\mathcal{U}$. When gravitational energy is included, the constant of A can be adjusted so that -A is equal to the sum of $\mathcal{U}$ and the total gravitational energy. This is done in what follows. In Section V it is shown that, for a stable static atmosphere, A is minimum and so the sum of $\mathcal{U}$ and the gravitational energy is maximum. In Section VII E it is shown that, in a relativistic context, the statement that $\mathcal{U}$ is maximum for stable flow holds even for arbitrary fluid motion. This statement is equivalent to the statement that the total entropy S is maximum for stable flow. This obviously is a Second Law definition of stability. In Section VI it is shown that the First Law form of the Principle of Virtual Work **cannot** be adapted to include fluid **motion.** Thus, whereas either the First-Law form or the Second-Law form of the Principle of Virtual Work can be used in the static case, only the Second-Law form can be extended to the dynamic case.

The fact that, in the static case, both forms of the Principle of Virtual Work constitute valid but different stability criteria provides the means for constructing a **minimax** statement of the problem, which in the case of a box of gas is simply the statement that U tends to a minimum whereas $\mathcal{U}$ tends to a maximum, and at equilibrium the two are equal. That is, if S is suppressed by making it constant throughout the box of gas, then it follows from Equation (37) that

$$U = \int_V u(n)\, d^3(x); \quad \mathcal{U} = \int_V [nH - P(H)]\, d^3(x)\,; \qquad (58a, b)$$

and, from the inequality of Equation (36), that

$$\int_V u(n)\, d^3(x) \geqslant \int_V [nH - P(H)]\, d^3(x)\,. \tag{58c}$$

This inequality could serve as the basis of a direct, iterative way of finding $\tilde{n}(x)$ and $\tilde{H}(x)$ in that a best answer for $n(x)$ is found by **minimizing** the **left** side, and then substituting this best answer into the right side a best answer for $H(x)$ is found by **maximizing** the **right** side. For this simple problem, these two steps would suffice to give $\tilde{n}(x)$ and $\tilde{H}(x)$, but in a more complicated minimax problem successive iterations might be necessary. It is important to note that $n(x)$ and $H(x)$ are varied **in turn, not simultaneously.** If they were varied simultaneously, then, because of the presence of the term nH in the integrand, it would no longer be possible to assert that $\tilde{U}$ = maximum since the sign of $\delta^{(2)}\tilde{U}$ would be indefinite. It would, however, be permissible to vary n and H simultaneously if the condition $\int \delta n \delta H\, d^3(x) \leqslant 0$ were observed. This is just a special case of the Second-Law condition stated in Equation (44).

The transition from a minimum principle to an equivalent maximum principle as illustrated in Equation (58) is called a Friedrichs transformation. It was developed by Friedrichs[2] in order to demonstrate the equivalence of the Dirichlet and Castigliano Principles. He also pointed out that, because the Castigliano Principle involves the intensive quantities of the problem as primitive variables rather than as derived quantities, it is usually easier to fit boundary conditions on a free boundary where intensive quantities have specified values. On the other hand, the convergence of a numerical solution is often faster using the Dirichlet Principle.

In order to generalize the above considerations from a simple box of gas to a static atmosphere in a gravitation field, it is only necessary to replace $u$ and $u$ with $(u + nM\phi)$

and ($u$ + nM$\phi$) respectively, where $\phi = \phi(x, t)$ is the specified gravitational potential. The corresponding total energy E and total internal free energy A are then

$$E = \int_V [u(n, S) + nM\phi(x,t)]\, d^3(x) \tag{59a}$$

$$= \int_N [U(\hat{V}, S) + M\phi(X, t)]\, d^3(\Lambda) \tag{59b}$$

and

$$A = -\int_V (u + nM\phi)\, d^3(x) \tag{60a}$$

$$= \int_V [P(H, S) - nM\phi - nH]\, d^3(x) \tag{60b}$$

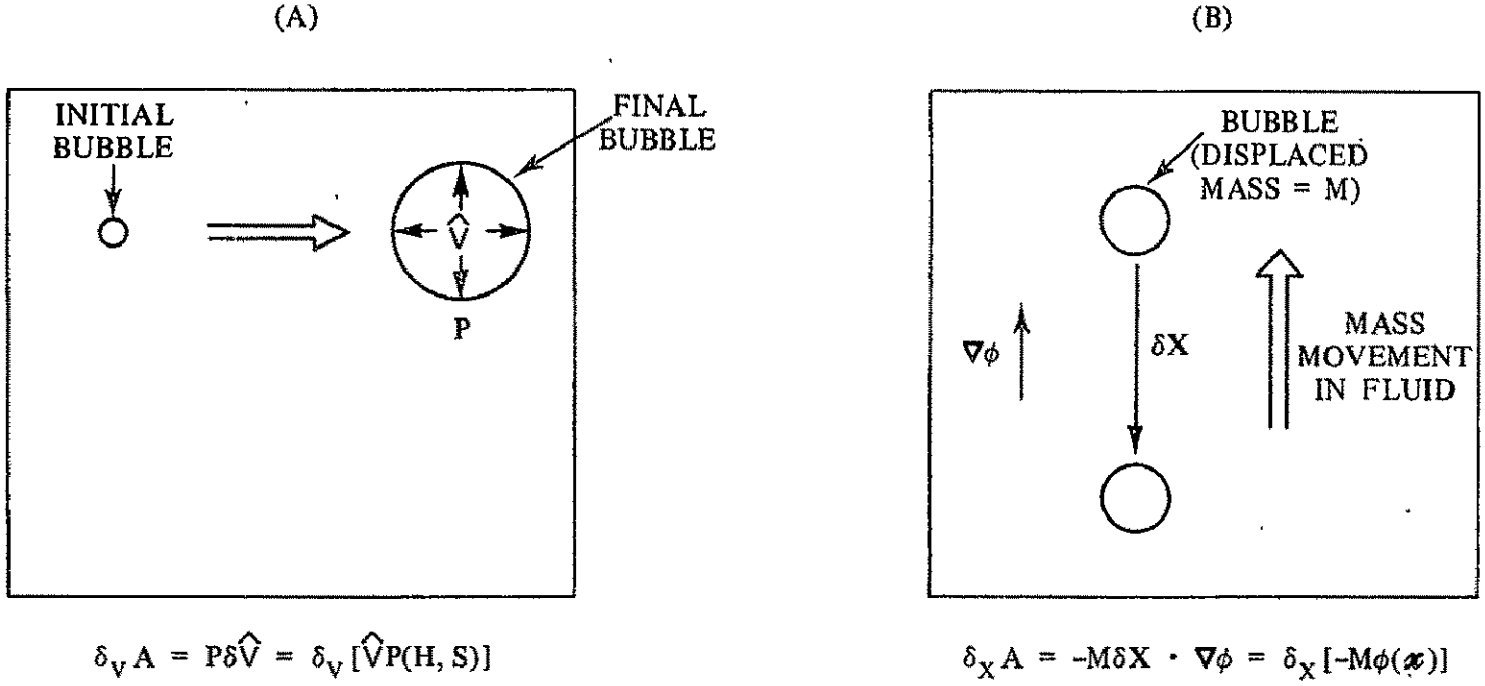
$$= \int_N [\hat{V}P(H, S) - M\phi - H]\, d^3(\Lambda)\,. \tag{60c}$$

In Sections IV and V it will be shown by direct calculation of the first and second variations that E and A are both minima for a stable static atmosphere.

It is evident from (60c) that, if H is parameterized in such a way that the variation of its integral is identically zero, then it could be omitted altogether and A could be identified with $\int (\hat{V}P - M\phi)\, dN$. If H is expressed as a Jacobian constructed on the three families of surfaces $\eta^A(\Lambda, t)$, i.e. if $H \equiv \det(\partial\eta^A/\partial\Lambda^B)$ and $\delta\eta^A = 0$ on those $\Lambda$-surfaces that coincide with the boundary (either free or rigid) of the system, then $\delta \int H\, dN = 0$ to all orders and H can be dropped from the integrand of Equation (60c). (In the case of an action integral over time as well as space, the same thing can be accomplished by representing H in the form $H \equiv (\partial_t \eta^o)_\Lambda$ where $\eta^o(\Lambda, t)$ replaces H as the primitive variable. If $\delta\eta^o = 0$ at $t_I$ and $t_F$, then $\delta[\int H\, dt]_\Lambda = 0$ to all orders.)

The intuitive significance of the energy $\hat{V}P - M\phi$ that survives in the integrand of Equation (60c) if H is dropped is illustrated in Figure 2. Figure 2A illustrates that $\hat{V}P$ is the energy required to inflate a bubble of volume $\hat{V}$ against a pressure P. This energy could be recovered by arranging to utilize the energy that would be delivered by the surrounding fluid during a quasi-static collapse of the bubble. Thus, although the energy resides in the surrounding fluid, its conversion to some other form occurs in or near the volume $\hat{V}$ and so is to be associated with this volume.

The corresponding interpretation in the case of gravitational energy is illustrated in Figure 2B. According to this interpretation, the energy of interest is the potential energy of a bubble embedded in the atmosphere. Since a bubble tends to rise rather than fall, the relevant potential energy is $-M\phi$ (if the bubble displaces one mole of fluid) rather than $+M\phi$ which would be the potential energy of one mole of isolated matter, rather than the energy of an embedded bubble. An alternative way to justify the same conclusion is to note that if the bubble is pushed downward a distance $\delta X$, a mole of matter in the surrounding fluid must be raised a corresponding distance, so the total potential energy of the atmosphere has been increased, and this increase in energy must be associated with a decrease in height (of the bubble). Here again, the energy resides outside the bubble, but because its conversion to some other form (usually kinetic energy) is a function of the change in bubble height, it must be associated with the bubble. Thus $(\hat{V}P - M\phi)$ is to be regarded as the potential energy of a bubble of volume $\hat{V}$ that displaces mass M. It can be shown that for a vertical column extending from the bottom to the top of a static atmosphere $\int(\hat{V}P - M\phi)\, dN = 0$ at equilibrium and increases for any fluctuation from equilibrium if the atmosphere is stable. Thus this integral can be considered the total buoyancy potential of the atmosphere, and this is the quantity that is to be identified with the total internal free energy A of a static atmosphere.




$$\delta_V A = P\delta\hat{V} = \delta_V [\hat{V}P(H, S)]$$

$$\delta_X A = -M\delta X \cdot \nabla\phi = \delta_X [-M\phi(x)]$$

Figure 2. Potential Energy of a Molar "Bubble". (A) Compressive Energy of a Bubble With Molar Volume. (B) Change in Gravitational Energy of a Bubble that Displaces Molar Mass.

In the sections that follow, the -H in the integrand of Equation (60c) will be retained. Its inclusion may be regarded simply as an arbitrary change in the reference level of the energy $(\hat{V}P - M\phi)$.

The fact that the molar **free energy** is effectively the energy of the corresponding **bubble** whereas the energy E is the **total energy** of the **matter within the bubble** is related to the fact that in a static atmosphere $\delta E$ is equal to the work done against the body force F that acts on the **matter**, whereas $\delta A$ is equal to the work done against the deformation force $\mathscr{D}$ that acts on the **bubble** containing the matter:

$$\delta E = -\mathbf{F} \cdot \delta X ; \quad (\delta A)_S = - \mathscr{D} \cdot \delta X ; \qquad (61a, b)$$

where, by Equation (10a), $\mathscr{D} = -F$ for a static atmosphere. These relations will be confirmed by the first-order variations calculated in Sections IV and V.

## IV. TOTAL ENERGY OF A STATIC ATMOSPHERE

Dirichlet's Principle applied to a static atmosphere says that the atmosphere is stable if the total thermal and gravitational energy is a minimum with respect to all possible fluctuations about the state of hydrostatic equilibrium. That is, for the equilibrium configuration the first variation of the total energy E of the atmosphere should vanish, and its second variation should be positive-definite. Thus

$$\delta^{(1)}E = 0 \quad \text{and} \quad \delta^{(2)}E > 0 \tag{62a, b}$$

are sufficient conditions for stability of a static atmosphere if the atmosphere is thermally isolated and the virtual fluctuations are isentropic. From the thermodynamic point of view, the above conditions are simply the standard way of characterizing a stable isolated system in the energy representation. (In the entropy representation the corresponding characterization is the statement that the total entropy of a stable isolated system is maximum.[11])

The most direct way[1] to obtain expressions for $\delta^{(1)}E$ and $\delta^{(2)}E$ in terms of the particle displacement $\delta X$ is to write $E = \int (U + M\phi)\, nd^3(x)$, and then use the relations $\delta n = -n\nabla \cdot \delta X$, $\delta\phi = \delta X \cdot \nabla\phi$, $(\delta U)_S = -(p/n)\, \nabla \cdot \delta X$, and similar thermodynamic relations to reduce all differentials to expressions involving $\delta X$. This approach shows that the condition $\delta^{(1)}E = 0$ is satisfied if the equation for hydrostatic equilibrium is satisfied, and that the condition $\delta^{(2)}E > 0$ is consistent with the Väisälä-Brunt stability criterion.[8,9] This form of proof could be termed "non-holonomic" in the sense that the particle positions themselves are never explicitly represented, but rather only their differential displacements $\delta X$. By contrast, the proof given below is "holonomic" in that the particle positions are represented in terms of the Lagrange surfaces $\Lambda^A(x, t)$, and the $\delta X$ that appears in the expressions below is not a primitive differential variable, but rather is short-hand for the second-order expression in $\delta\Lambda^A$ that was given in Equation (36) of Paper I.

Although the mathematics involved in a holonomic calculation of $\delta^{(1)}E$ and $\delta^{(2)}E$ is far more intricate than in a non-holonomic calculation, the holonomic approach has the great advantage that it establishes the basis for a direct (i.e. trial-and-error) solution of complicated fluid-dynamical problems. Only after the action integral of a variational minimum principle has been expressed as an **explicit functional** is it possible to insert parameterized trial functions and adjust the parameters so as to minimize the integral. It is a treacherous fallacy to think that, once a variational minimum principle has been justified by a non-holonomic argument, it is a simple and straight-forward matter to write down the appropriate holonomic form of the action integral. This view is fallacious because it is possible to write down many different action integrals that are all identical for their common extremal flow, but which differ for non-extremal flows and, hence have radically different topologies in parameter space.

In the convected frame the independent variables are $\Lambda^A$, and if these are normalized in the manner described in Section II A of Paper I, then $d^3(\Lambda) = dN$ is the infinitesimal mole number and the explicit functional for E is

$$E = \int_N [U(\hat{V}, S) + M\phi(X, t)]\, d^3(\Lambda) \tag{63a}$$

where the trial functions are the three components of $X(\Lambda^A, t)$ and the functional dependence of $\phi(X, t)$ is given. (X will be used to designate the dependent vector function $X(\Lambda, t)$ whereas $\boldsymbol{x}$ will be used to designate the corresponding position vector used as an independent coordinate.) The time dependence of $\phi$ and X (and of S, if such is specified) is to be regarded merely as a parametric dependence since in Sections IV and V time is not included among the independent variables. Its inclusion makes no difference in the calculated expressions given below for the variations. The molar volume $\hat{V}$ and the molar entropy S

are given by

$$\hat{V} \equiv J^{X}_{\Lambda} \equiv \det\left(\frac{\partial X^{j}}{\partial \Lambda^{A}}\right); \quad S = S(\Lambda^{A}, t); \tag{63b, c}$$

where $S(\Lambda, t)$ is a specified function. The molar equilibrium internal energy $U(\hat{V}, S)$ is also known, either as an explicit function as illustrated in Equation (49) for a perfect gas, or as an expansion of the type illustrated in Equation (55) for the case of an arbitrary fluid.

In a Cartesian inertial frame, E has the form

$$E = \int_{V} [u(n, S) + nM\phi(x, t)]\, d^{3}(x) \tag{64a}$$

where now the trial functions are $\Lambda^{A}(\boldsymbol{x}, t)$, $(A = 1, 2, 3)$ and

$$n \equiv J^{\Lambda}_{x} = \det\left(\frac{\partial \Lambda^{A}}{\partial x^{j}}\right); \quad S = S[\Lambda^{A}(\boldsymbol{x}, t); t]\ . \tag{64b, c}$$

$S(\Lambda, t)$ is the same specified function as given in Equation (63c), but now it is a function of $\boldsymbol{x}$ and t because of the $(\boldsymbol{x}, t)$–dependence of $\Lambda^{A}(\boldsymbol{x}, t)$. $\phi(\boldsymbol{x}, t)$ is the same specified function that appears in Equation (63a), and the equilibrium internal energy density $u(n, S) = nU$ is either a known function of n and S of the type illustrated in Equation (50) for a perfect gas, or else of the expansion type illustrated in Equation (56) for an arbitrary fluid.

For the reasons discussed in Section III A of Paper I, the calculation of $\delta^{(1+2)}E$ was carried out in the inertia frame rather than in the convected frame. The necessary expression for $\delta^{(1+2)}n$ is given in Equations (15) and (16) above, or in Equation (44) of Paper I. The expression for $\delta^{(1+2)}S$ is given in Equation (4) above, or Equation (43) of Paper I. Using these expressions, together with Equations (7) and (53), the expression for $\delta^{(1+2)}E$ can,

after much partial integration and algebraic manipulation, be cast into the following form:

$$\delta^{(1+2)}E = [\delta^{(1+2)}E]_S + \sum_{N=1}^{3} [\delta^{(1+2)}E]_V^{(N)} \tag{65a}$$

where

$$[\delta^{(1+2)}E]_S = -\int_{\mathscr{S}} [(\bar{H} + M\bar{\phi}) - \tfrac{1}{2}\delta X \cdot \nabla(\bar{H} + M\bar{\phi}) - \tfrac{1}{2}\delta X \cdot \bar{F}_p]\, \delta^{(1+2)}n \cdot d\mathscr{S}; \tag{65b}$$

$$[\delta^{(1+2)}E]_V^{(1)} = -\int_V \bar{F}_p \cdot \delta^{(1+2)}n\, d^3(x); \tag{65c}$$

$$[\delta^{(2)}E]_V^{(2)} = \int_V \tfrac{1}{2}\bar{\beta}[(\nabla \cdot \delta X) + \frac{1}{\bar{\beta}}(\delta X \cdot \nabla\bar{p})]^2\, d^3(x); \tag{65d}$$

$$[\delta^{(2)}E]_V^{(3)} = \int_V \tfrac{1}{2}[(\delta X \cdot \nabla \ell n\, \bar{n})(\delta X \cdot \nabla\bar{p}) - \frac{1}{\bar{\beta}}(\delta X \cdot \nabla\bar{p})^2]\, d^3(x); \tag{65e}$$

where $\delta^{(1+2)}n$ is given in Equation (15) and

$$\bar{F}_p \equiv -\frac{1}{\bar{n}}\nabla\bar{p} - M\nabla\bar{\phi};\quad \bar{H} \equiv \overline{(\partial u/\partial n)}_S; \tag{65f, g}$$

$$\bar{p} \equiv \overline{nH} - \bar{u};\quad \bar{\beta} \equiv \bar{n}^2\left(\overline{\frac{\partial^2 u}{\partial n^2}}\right)_S. \tag{65h, i}$$

The subscript p has been added to $\bar{F}_p$ to emphasize that in this case the force involves $\nabla p$ rather than $\nabla P$, which will be encountered in Sections V and VII. The overhead bar indicates the $(\boldsymbol{x}, t)$-dependence that corresponds to the particular set of trial functions $\bar{\Lambda}^A(\boldsymbol{x}, t)$ about which the variation takes place. These are **not** assumed to be the **extremal** trial functions, which will be designated $\tilde{\Lambda}^A(\boldsymbol{x}, t)$. The extremal trial functions are the ones for which $[\delta^{(1)}\tilde{E}]_V = 0$. This in turn requires that $-\tilde{F}_p = \frac{1}{\tilde{n}}\nabla\tilde{p} + M\nabla\tilde{\phi} = 0$, which is the hydrostatic force equation. Thus the integral given in Equation (65c) vanishes in the extremal case. A comparison with Equation (61a) shows that in the general

non-extremal case the integral of Equation (65c) represents the work that is being done against the non-vanishing force $\overline{\mathbf{F}}_p$ by the displacement flux $\delta^{(1+2)}\mathbf{n}$.

The integral given in Equation (65e) is the spatial integral of the Väisälä-Brunt expression for the buoyancy displacement work that was given in Equation (27). The integrand of Equation (65e) is a slight generalization of the expression in Equation (27) in that Equation (65e) is not limited to displacements from hydrostatic equilibrium, but rather represents the second-order change in energy resulting from a displacement from an arbitrary non-equilibrium state of the atmosphere. (The first-order energy change is included in the integral of Equation (65c).)

The integral given in Equation (65d) represents the energy increase that results from any deviation from equality between internal and external pressures. This can be seen by writing the integrand of Equation (65d) in the form

$$\tfrac{1}{2}\overline{\beta}[(\nabla \cdot \delta\mathbf{X}) + \frac{1}{\overline{\beta}}(\delta\mathbf{X} \cdot \nabla\overline{p})]^2 = \tfrac{1}{2}\overline{n}\,\overline{U}_{VV}[\delta_X\hat{V} - (\delta_p\hat{V})_S]^2 \qquad (66a)$$

where $\delta_X\hat{V} = \hat{V}\nabla \cdot \delta\mathbf{X}$ and $(\delta_p\hat{V})_S$ is the adiabatic change in molar volume that corresponds to a change in internal pressure that is equal to the change $\delta\mathbf{X} \cdot \nabla\overline{p}$ in external pressure, i.e.

$$(\delta_p\hat{V})_S \equiv \overline{\left(\frac{\partial\hat{V}}{\partial p}\right)_S}\,\delta\mathbf{X} \cdot \nabla\overline{p} = -\frac{\overline{\hat{V}}}{\overline{\beta}}\,\delta\mathbf{X} \cdot \nabla\overline{p} \qquad (66b)$$

where use has been made of the definition of $\beta$ given in Equation (21). Because $(\delta_V^{(2)}U) = \tfrac{1}{2}\overline{U}_{VV}(\delta\hat{V})^2 \equiv \tfrac{1}{2}(\partial^2 U/\partial\hat{V}^2)_S\,(\delta\hat{V})^2$ is the second-order change in molar internal energy that is produced by an adiabatic volume change, it is evident that Equation (66a) represents the density of energy change that is to be associated with the adiabatic deviation of $\delta_X\hat{V}$ from the pressure-equalizing volume change $(\delta_p\hat{V})_S$.

The surface integral in Equation (65b) represents the loss in energy by transport of matter across the fixed bounding surface. The energy lost per mole of matter that leaves V is $\bar{H} + M\bar{\phi}$. The term $-\frac{1}{2}\delta X \cdot \nabla(\bar{H} + M\bar{\phi})$ is the correction that results because at the end of the displacement $\delta X$ the matter at the observation point $x$ on the surface $\mathcal{S}$ was originally at $x - \delta X$, and the factor ½ gives the average between beginning and end of the displacement. The term $-\frac{1}{2}\delta X \cdot \bar{F}$ represents the amount that the energy of the lost matter had been increased because of work against the force $\bar{F}_p$. If the standard boundary conditions given in Equation (54) of Paper I are imposed, it follows that $\delta^{(1+2)}n \cdot d\mathcal{S} = 0$, and the surface integral vanishes.

Imposing these boundary conditions, and replacing the integrand of Equation (65e) with the equivalent expression given in Equation (32), it is evident that at the extremum the variation of E is a purely second-order expression:

$$\delta^{(1+2)}\tilde{E} = \delta^{(2)}\tilde{E} = \tfrac{1}{2}\int_V \tilde{\beta}\left[(\nabla \cdot \delta X) + \frac{1}{\tilde{\beta}}(\delta X \cdot \nabla\tilde{p})\right]^2 d^3(x) - \tfrac{1}{2}\int_V \left(\frac{\tilde{\gamma}-1}{\tilde{\alpha}\tilde{\beta}}\right)[(\nabla\tilde{S}\nabla\tilde{p}):\delta X\delta X]\,\tilde{n}\,d^3(x)\,. \tag{67}$$

This is the expression that resulted from Eliassen's[1] non-holonomic derivation. (His expression replaces $\nabla\tilde{p}$ with $-\tilde{n}M\nabla\tilde{\phi}$, but this is valid only in the static case, whereas Equation (67) continues to be valid in the dynamic case considered in Section VI for which $\tilde{D}_t\tilde{V} \neq 0$.)

## V. TOTAL INTERNAL FREE ENERGY OF A STATIC ATMOSPHERE

The heuristic arguments of Section III indicated that the Second-Law or Castigliano form of the Principle of Virtual Work corresponds to variations of a total internal free energy A of the form given in Equation (60). In this Section, an integral functional of this form will be taken as the starting point, and the general expression for the first and second variations about an arbitrary set of trial functions (indicated by an overhead bar) will be calculated. It will be shown that $\delta^{(1+2)}A$ has just the form to be expected for the variation of a free energy, namely a differential work minus the accompanying differential increase in heat or unavailable energy.

When expressed in the convected frame, the total free energy will be defined to be

$$A = \int_N [\hat{V}P(H, S) - M\phi(\boldsymbol{x}, t) - H(\Lambda, t)]\, d^3(\Lambda) \tag{68a}$$

where $\phi(\boldsymbol{x}, t)$ and $S(\Lambda, t)$ are prescribed functions, $\hat{V} \equiv J^X_\Lambda$, and P(H, S) is a known state function. Compared with Equation (63), an additional degree of freedom is present in the undetermined functional dependence of $H(\Lambda, t)$ whose variation is represented by

$$H(\Lambda, t) = \bar{H}(\Lambda, t) + \delta_H H\,. \tag{68b}$$

In a Cartesian inertial frame A has the form

$$A = \int_V [P(H, S) - nM\phi(x, t) - nH(\Lambda, t)]\, d^3(x)\,. \tag{69a}$$

Like $S = S[\Lambda^A(\boldsymbol{x}, t); t]$, H varies by virtue of the variations of its argument functions $\Lambda^A(\boldsymbol{x}, t)$. However, it has an additional variation because its functional dependence on these argument functions is not specified. As indicated in Equation (40), its total variation about an arbitrarily chosen set of trial functions $\bar{\Lambda}^A(\boldsymbol{x}, t)$ is

$$\delta^{(1+2)}H \equiv H[\Lambda^A(\boldsymbol{x}, t); t] - \bar{H}[\bar{\Lambda}^A(\boldsymbol{x}, t); t]$$

$$= -\delta X \cdot \nabla\bar{H} + \tfrac{1}{2}(\delta X \delta X : \nabla\nabla\bar{H}) \tag{69b}$$

$$+ \delta_H H - \delta X \cdot \nabla(\delta_H H) .$$

The expressions for $\delta^{(1+2)}S$ and $\delta^{(1+2)}n$ are given in Equations (4), (15) and (16). The first and second partials of P(H, S) are given in Equations (33) and (54). Using these, the expression for the first and second variations of A in the inertial frame can, after considerable reduction, be cast into the following form:

$$\delta^{(1+2)}A = [\delta^{(1+2)}A]_S + \sum_{N=1}^{5} [\delta^{(1+2)}A]_V^{(N)} \tag{70a}$$

where

$$[\delta^{(1+2)}A]_S = \int_{\mathscr{S}} [(\bar{H} + M\bar{\phi}) - \tfrac{1}{2}\delta X \cdot \nabla(\bar{H} + M\bar{\phi}) - \tfrac{1}{2}\delta X \cdot \bar{F}_P - \frac{\bar{N}}{\bar{n}} \delta_H H]\, \delta^{(1+2)}\mathbf{n} \cdot d\mathscr{S}; \tag{70b}$$

$$[\delta^{(1+2)}A]_V^{(1)} = \int_V \bar{F}_P \cdot \delta^{(1+2)}\mathbf{n}\, d^3(x) ; \tag{70c}$$

$$[\delta^{(1)}A]_V^{(2)} = \int_V (\bar{N} - \bar{n})\, \delta_H H\, d^3(x) ; \tag{70d}$$

$$[\delta^{(2)}A]_V^{(3)} = \int_V \frac{1}{2\bar{\beta}} (\bar{N}\delta_H H + \bar{\beta}\nabla \cdot \delta X)^2\, d^3(x) ; \tag{70e}$$

$$[\delta^{(2)}A]_V^{(4)} = \int_V \tfrac{1}{2}[(\delta X \cdot \nabla \ell n\, \bar{n})(\delta X \cdot \nabla\bar{P}) - \bar{\beta}(\nabla \cdot \delta X)^2]\, d^3(x); \tag{70f}$$

$$[\delta^{(2)}A]_V^{(5)} = -\int_V (\delta^{(1)}n)\, [\delta_H H - \delta X \cdot \nabla\bar{P}/\bar{n}]\, d^3(x) ; \tag{70g}$$

where $\delta^{(1+2)}\mathbf{n}$ is given in Equation (15) and

$$\bar{F}_P \equiv -\frac{1}{\bar{n}} \nabla\bar{P} - M\nabla\phi ; \tag{70h}$$

$$\bar{N} \equiv \overline{(\partial P/\partial H)_S} \; ; \; \bar{\beta} \equiv \left[\frac{\overline{(\partial P/\partial H)_S^2}}{(\partial^2 P/\partial H^2)_S}\right] = \frac{\bar{N}^2}{\bar{P}_{HH}} \; . \qquad (70i, j)$$

The sum $[\delta^{(1+2)}A]_V^{(1)} + [\delta^{(1+2)}A]_V^{(2)}$ is just equal to the spatial integral of $\delta^{(1+2)}a$ given in Equation (47b) (for $\bar{D}_t\bar{V} = 0$). Thus these two integrals represent the change in free deformation energy to be associated with $\bar{F}_P \neq 0$ and $\bar{N} - \bar{n} \neq 0$. The sum $[\delta^{(2)}A]_V^{(4)} + [\delta^{(2)}A]_V^{(5)}$ is equal to the integral given in Equation (48b) (except that it is not limited to displacements from equilibrium). Thus this sum is the change in free energy to be associated with the buoyancy restoring force.

The integral $[\delta^{(2)}A]_V^{(3)}$ can be interpreted as the second-order change in the internal energy density that results because of the discrepancy between $(\delta_H N)_S$, the change in (intensive) mole density produced by an isentropic change in enthalpy, and $\delta_X N \equiv -N\nabla \cdot \delta\mathbf{X}$, which is the amount by which the intensive mole density would change if its change were consistent with $\nabla \cdot \delta\mathbf{X}$. This interpretation follows from the fact that $(\delta_H N)_S \equiv (\partial N/\partial H)_S \; \delta_H H = P_{HH}\delta_H H = \dfrac{N^2}{\beta}\delta_H H$ where in the last step use has been made of Equation (70j). If $u(N, S)$ is the internal energy density that corresponds to the intensive mole density N, then Equation (53) shows that $u_{NN} = \beta/N^2$ where the $\beta$ is the same intensive bulk modulus that is defined in Equation (70j). Using these relations, the integrand of Equation (70e) can be written in the following form:

$$\begin{aligned} \frac{1}{2\bar{\beta}}(\bar{N}\delta_H H + \bar{\beta}\nabla \cdot \delta\mathbf{X})^2 &= \tfrac{1}{2}\frac{\bar{\beta}}{\bar{N}^2}\left(\frac{\bar{N}^2}{\bar{\beta}}\delta_H H + \bar{N}\nabla \cdot \delta\mathbf{X}\right)^2 \\ &= \tfrac{1}{2}\bar{u}_{NN}[(\delta_H N)_S - (\delta_X N)]^2 \equiv \delta^{(2)}_{(H,X)}u \; . \end{aligned} \qquad (71)$$

If the enthalpy change in a sample of the fluid is purely in accord with equilibrium adiabatic expansion or compression, then $(\delta_H N)_S = (\delta_X N)$ and the change in energy density given by Equation (71) vanishes. This energy is therefore the non-negative energy increase

that results from the non-adiabatic fluctuating transport of thermal energy through the fluid, i.e. the random "sloshing about" of heat flux. In an inviscid turbulent fluid this heat flux could also be pictured as including the "quasi-heat flux" of randomized isotropic turbulence energy.

The energy density represented in Equation (71) should be regarded as supplementing the buoyancy energy density $\bar{n}(\delta^{(2)}A)_S$ which appears in the integrand of Equation (70f). [$(\delta^{(2)}A)_S$ is the expression given in Equation (25), with bars replacing the tildes.] The derivation of Equation (25) showed that this expression is the work of an **adiabatic** displacement $\delta\mathbf{X}$, whereas $\delta^{(2)}_{(H,\,X)}u$ is the energy change resulting from heat flux that accompanies the displacement. Thus the integrals of Equations (70e) and (70f) taken together represent the total energy increase to be associated with the displacement field $\delta\mathbf{X}$. Equations (42b) and (44) show that the integral of Equation (70g) is just the negative of the increase in unavailable energy that accompanies the displacement $\delta\mathbf{X}$. Thus the sum of the three integrals given in Equations (70e–70g) is just the total (second-order) change in free energy that is produced by the displacement field $\delta\mathbf{X}$ and the simultaneous change in molar enthalpy $\delta_H H$.

In a similar way, the sum of the integrals given in Equations (70c) and (70d) represents the change in free energy that, unlike the change discussed above, is of **first** order in $\delta\mathbf{X}$ and $\delta_H H$ (with a second-order contribution $\bar{\mathbf{F}}_p \cdot \delta^{(2)}\mathbf{n}$). This is seen by noting that it follows from Equation (14) that for a static atmosphere ($D_t V = 0$), $\bar{\mathbf{F}}_p \cdot \delta^{(1\,+\,2)}\mathbf{n} = -\bar{\mathscr{D}} \cdot \delta^{(1\,+\,2)}\mathbf{n} = (\delta^{(1\,+\,2)}a)_S$ is just the isentropic deformation work that is performed by the displacement flux $\delta^{(1\,+\,2)}\mathbf{n}$ against the deformation force $\bar{\mathscr{D}}$. Equation (42a) shows that the integral given in Equation (70d) is just the negative of the unavailable energy increase that results from the enthalpy change $\delta_H H$.

Thus, if the standard boundary conditions are imposed, the surface integral given in Equation (70b) vanishes, and the total variation of A can be written in the following form:

$$\delta^{(1+2)}A = \int_V [(\delta^{(1+2)}a)_S - \bar{n}\delta_H Q]\, d^3(x) + \int_V [\delta^{(2)}_{(X,H)}u + \bar{n}(\delta^{(2)}A)_S - (\delta^{(1)}n)\,\delta_X Q]\, d^3(x) \tag{72a}$$

where

$$(\delta^{(1+2)}a)_S \equiv -\bar{\mathscr{D}} \cdot \delta^{(1+2)}\mathbf{n} = -\left(\frac{1}{\bar{n}}\nabla\bar{P} + M\nabla\bar{\phi}\right) \cdot \delta^{(1+2)}\mathbf{n}\,; \tag{72b}$$

$$\delta_H Q \equiv \left(1 - \frac{\bar{N}}{\bar{n}}\right)\delta_H H\,; \tag{72c}$$

$$\delta^{(2)}_{(X,H)}u \equiv \tfrac{1}{2}\bar{u}_{NN}[(\delta_H N)_S - (\delta_X N)]^2 = \tfrac{1}{2}\frac{\bar{\beta}}{\bar{N}^2}\left(\frac{\bar{N}^2}{\bar{\beta}}\delta_H H + \bar{N}\nabla\cdot\delta X\right)^2\,; \tag{72d}$$

$$(\delta^{(2)}A)_S \equiv \frac{1}{2\bar{n}}[(\delta X\cdot\nabla\ell n\,\bar{n})(\delta X\cdot\nabla\bar{P}) - \bar{\beta}(\nabla\cdot\delta X)^2]\,; \tag{72e}$$

$$\delta_X Q \equiv \delta_H H - \delta X\cdot\nabla\bar{P}/\bar{n}\,; \tag{72f}$$

$$\delta^{(1)}n = -\nabla\cdot(\bar{n}\delta X)\,;\quad \bar{N} \equiv \left(\overline{\frac{\partial P}{\partial H}}\right)_S\,;\quad \bar{\beta} \equiv \frac{\bar{N}^2}{\overline{P_{HH}}}. \tag{72g, h, i}$$

Both integrals on the right side of (72a) have the form of changes in free energy. The first integral vanishes in the extremal case which is characterized by

$$\tilde{\mathscr{D}} = \frac{1}{\tilde{n}}\nabla\tilde{p} + M\nabla\tilde{\phi} = 0\,;\quad \tilde{N} = \tilde{n}. \tag{73a, b}$$

(Use has been made of the fact that $\tilde{N} = \tilde{n}$ implies $\tilde{P} = \tilde{p}$.) The second-order variation of A around the extremal solution, $\delta^{(2)}\tilde{A}$, is given by the second integral on the right side of Equation (72a) with the bars replaced by tildes and $\bar{P}$ and $\bar{N}$ replaced by $\tilde{p}$ and $\tilde{n}$.

Adiabatic displacements about the extremal solution are characterized by the condition

$$\delta_X \tilde{Q} = \delta_H H - \delta X \cdot \nabla\tilde{p}/\tilde{n} = 0 . \tag{74}$$

When $\delta_H H = \delta X \cdot \nabla\tilde{p}/\tilde{n}$ is substituted into Equation (70e) this becomes identical to Equation (65d), i.e.

$$[\delta^{(2)}\tilde{A}]_V^{(3)} = [\delta^{(2)}\tilde{E}]_V^{(2)} \text{ for } \delta_X \tilde{Q} = 0 . \tag{75}$$

The following condition on $\delta X$ must be fulfilled if the adiabatic change in internal pressure that is produced by a volume change, $(\delta_V \tilde{p})_S$, is to be equal to the change in external pressure $\delta X \cdot \nabla\tilde{p}$: $(\delta_V \tilde{p})_S \equiv \tilde{\beta}\nabla \cdot \delta X = \delta X \cdot \nabla\tilde{p}$. If $\nabla \cdot \delta X = (\delta X \cdot \nabla\tilde{p})/\tilde{\beta}$ is substituted into Equation (70f), it becomes equal to Equation (65e), i.e.

$$[\delta^{(2)}\tilde{A}]_V^{(4)} = [\delta^{(2)}\tilde{E}]_V^{(3)} \text{ for } \tilde{\beta}\nabla \cdot \delta X = \delta X \cdot \nabla\tilde{p} . \tag{76}$$

If the fluctuations in A observe the conditions of Equations (74) and (76) simultaneously, then

$$\delta^{(2)}\tilde{A} = \delta^{(2)}\tilde{E} \tag{77a}$$

if

$$\delta_H H = \delta X \cdot \nabla\tilde{p}/\tilde{n} \text{ and } \tilde{\beta}\nabla \cdot \delta X = \delta X \cdot \nabla\tilde{p} . \tag{77b, c}$$

In other words, because A involves an extra degree of freedom represented by the inclusion of H as an independent variable, a wider class of fluctuations is possible compared with the fluctuations of E. However, the subclass of A-fluctuations that is adiabatic and pressure-equalizing is identical to the class of E-fluctuations, and for this subclass the variations in A and E about their common extremum are identical.

This statement is valid only if the standard boundary conditions given in Equation (54) of Paper I are satisfied. If, however, these conditions are not imposed and matter is allowed to cross the boundary, then

$$[\delta^{(1+2)}\tilde{A}]_S = -[\delta^{(1+2)}\tilde{E}]_S \text{ if } \delta_H H = 0 \text{ on } \mathscr{S} . \tag{78}$$

This is the surface counterpart of the non-extremal volume relation

$$[\delta^{(1)}A]_V = -[\delta^{(1)}E]_V \text{ if } \bar{n} = \bar{N} \text{ in } V . \tag{79}$$

The reason for this difference in sign is evident from a comparison of Equations (59a) and (60a). Except for the subtle (but important) difference between $u$ and $u^*$, A is defined to be just the negative of E, and at the extremum this is exactly the case:

$$\tilde{A} = -\tilde{E} . \tag{80}$$

The physical explanation of this sign difference is that A is a potential function for the work done **on the environment** of every sample of matter under consideration, whereas E is a potential function for the work done **on the matter itself.**

## VI. IRREDUCIBLE FORM OF HAMILTON'S PRINCIPLE

With the explicit expression for $\delta^{(1+2)}\mathscr{H}$ given in Section IV of Paper I, and the expressions for $\delta^{(1+2)}E$ and $\delta^{(1+2)}A$ that were derived in Sections IV and V of this paper, it is possible to demonstrate the validity of two different forms of Hamilton's Principle for compressible baroclinic flow of an inviscid fluid in the presence of a given gravitational field. These two principles differ in the number of dependent variables involved, i.e. in the size of the set of trial functions involved. In the form of Hamilton's Principle presented in this section (whose first variation in the convected frame has long since been discussed in the literature[16-19]), three dependent variables are involved. In the convected-frame analysis these are the three components of the position vector $X(\Lambda^A, t)$ of the particle that is identified by the three Lagrange parameters $\Lambda^A$. In an inertial frame analysis the dependent variables are the three families of Lagrange surfaces $\Lambda^A(x, t)$. Either of these two sets of three functions constitutes the absolute minimum number of variables necessary to describe arbitrary three-dimensional flow, and for this reason the form of Hamilton's Principle that involves no more than these variables will be called the "irreducible form."

The irreducible action integral $\mathcal{L}$ and the total instantaneous Lagrangian L are defined in terms of the total kinetic energy W and the total static energy E by the following relations:

In the convected and inertial frames L is defined in terms of the molar Lagrangian L and the Lagrangian density $\ell$ respectively by the following relations:

$$L = \int_N L\,d^3(\Lambda) = \int_V \ell\,d^3(x) \tag{81b}$$

where

$$L = W - U(\hat{V}, S) - M\phi(X, t); \quad W \equiv \tfrac{1}{2}M(\partial_t X)_\Lambda \cdot (\partial_t X)_\Lambda \; ; \qquad (81c, d)$$

$$\ell = nW - u(n, S) - nM\phi(X, t); \quad W = \tfrac{1}{2}MV \cdot V \qquad (81e, f)$$

where

$$V = -\sum_{A=1}^{3} (\partial_t \Lambda^A)_x \, (\nabla\Lambda^B \times \nabla\Lambda^C)/n \, . \quad (A, B, C \text{ cyclic}) \qquad (81g)$$

In the convected frame $\hat{V} \equiv J^X_\Lambda$, and in a Cartesian inertial frame $n \equiv J^\Lambda_x$.

The expression for $\delta^{(1+2)}\mathscr{W}$ that was given in Equation (48) of Paper I can be put into a more compact form by making use of the identity

$$(\bar{n} + \delta^{(1)}n)\,\delta X \cdot \bar{A} - \tfrac{1}{2}\bar{n}(\delta X \delta X : \nabla \bar{A}) = \bar{A} \cdot \delta^{(1+2)}n - \nabla \cdot [\delta^{(1+2)}n(\tfrac{1}{2}\delta X \cdot \bar{A})] \qquad (82)$$

which is valid for any vector $\bar{A}$. When $\bar{A}$ is identified with the acceleration $\bar{D}_t\bar{V} \equiv \partial_t\bar{V} + \bar{V} \cdot \nabla\bar{V}$ for any set of trial functions, the sum of the integrals given in Equations (48d and e) of Paper I can be replaced by the following expression:

$$[\delta^{(1)}\mathscr{W}]_V + [\delta^{(2)}\mathscr{W}]^{(1)}_V = -\int_{(V, \Delta t)} M(\bar{D}_t\bar{V}) \cdot \delta^{(1+2)}n \, d^3(x) \, dt + \int_{(\mathscr{S}, \Delta t)} (\tfrac{1}{2}M\bar{D}_t\bar{V}) \cdot \delta X(\delta^{(1+2)}n) \cdot d\mathscr{S} dt \, . \qquad (83)$$

When the surface term of this equation is absorbed into the surface term given in Equation (48c) of Paper I, the following expression for $\delta^{(1+2)}\mathscr{W}$ results:

$$\delta^{(1+2)}\mathscr{W} = [\delta^{(1+2)}\mathscr{W}]_T + [\delta^{(1+2)}\mathscr{W}]_S + [\delta^{(1+2)}\mathscr{W}]_V \qquad (84a)$$

where

$$[\delta^{(1+2)}\mathscr{W}]_T = \int_N [M\bar{V} \cdot (\delta X + \delta X \cdot \nabla\delta X)]^{t_F}_{t_I} \, d^3(\bar{\Lambda}) \qquad (84b)$$

where $d^3(\Lambda) \equiv n\,d^3(x)$;

$$[\delta^{(1+2)}\mathscr{W}]_S = -\int_{(\mathscr{S},\Delta t)} [\overline{W} - \tfrac{1}{2}\delta X \cdot \nabla\overline{W} + \overline{D}_t(M\overline{V}\cdot\delta X) - \tfrac{1}{2}M(\overline{D}_t\overline{V})\cdot\delta X]\ \delta^{(1+2)}n \cdot d\mathscr{S}dt\,; \quad (84c)$$

$$[\delta^{(1+2)}\mathscr{W}]_V = -\int_{(V,\Delta t)} M(\overline{D}_t\overline{V}) \cdot \delta^{(1+2)}n\, d^3(x)\, dt + \int_{(V,\Delta t)} [\delta_t^{(2)}\overline{W} + \delta_X^{(2)}\overline{W}]\,\overline{n}\, d^3(x)\, dt \quad (84d)$$

where

$$\delta_t^{(2)}\overline{W} \equiv \tfrac{1}{2}M(\overline{D}_t\delta X)\cdot(\overline{D}_t\delta X)\,; \quad (84e)$$

$$\delta_X^{(2)}\overline{W} \equiv \tfrac{1}{2}M\delta X\delta X:[\nabla(\overline{D}_t\overline{V}) - (\nabla\nabla\overline{V})\cdot\overline{V}]\,. \quad (84f)$$

It can be shown that, if the terminal conditions $\delta X = 0$ at $t_I$ and $t_F$ are imposed, the term $\overline{D}_t(M\overline{V}\cdot\delta X)$ that appears in the integrand of Equation (84c) makes no net contribution to $[\delta^{(1+2)}\mathscr{W}]_S$, and so can be dropped.

The expression for $\delta^{(1+2)}\mathscr{L}$ follows from Equations (65) and (84):

$$\delta^{(1+2)}\mathscr{L} = \delta^{(1+2)}\mathscr{W} - \int_{t_I}^{t_F} \delta^{(1+2)}E\, dt = [\delta^{(1+2)}\mathscr{W}]_T + [\delta^{(1+2)}\mathscr{L}]_S + \sum_{N=1}^{3} [\delta^{(1+2)}\mathscr{L}]_V^{(N)} \quad (85a)$$

where $[\delta^{(1+2)}\mathscr{W}]_T$ is given by Equation (84b) and

$$[\delta^{(1+2)}\mathscr{L}]_S = -\int_{(\mathscr{S},\Delta t)} [(\overline{L} - \overline{p}/\overline{n}) - \tfrac{1}{2}\delta X\cdot\nabla(\overline{L} - \overline{p}/\overline{n}) + \overline{D}_t(M\overline{V}\cdot\delta X) - \tfrac{1}{2}\overline{\mathscr{D}}_p\cdot\delta X]\ \delta^{(1+2)}n\cdot d\mathscr{S}dt\,; \quad (85b)$$

$$[\delta^{(1+2)}\mathscr{L}]_V^{(1)} = -\int_{(V,\Delta t)} \overline{\mathscr{D}}_p \cdot \delta^{(1+2)}n\, d^3(x)\, dt\,; \quad (85c)$$

$$[\delta^{(2)}\mathcal{L}]_V^{(2)} = \tfrac{1}{2}M \int_{(V,\,\Delta t)} [(\bar{D}_t \delta X)\cdot(\bar{D}_t \delta X) - \bar{C}^2(\nabla\cdot\delta X + \delta X\cdot\nabla\bar{p}/\bar{\beta})^2]\,\bar{n}\,d^3(x)\,dt; \tag{85d}$$

$$[\delta^{(2)}\mathcal{L}]_V^{(3)} = \int_{(V,\,\Delta t)} (\delta_X^{(2)}\bar{W} - \delta^{(2)}\bar{A}_{VB})\,\bar{n}\,d^3(x)\,dt \tag{85e}$$

where

$$\bar{\mathscr{D}}_p \equiv -(\bar{F}_p - M\bar{D}_t\bar{V}) = M\bar{D}_t\bar{V} + \frac{1}{\bar{n}}\nabla\bar{p} + M\nabla\bar{\phi}. \tag{85f}$$

$\bar{C}$ is the speed of sound introduced via the relation $\bar{\beta} = \bar{n}M\bar{C}^2$; $\delta_X^{(2)}W$ is defined in Equation (84f); and $\delta^{(2)}\bar{A}_{VB}$ is the Väisälä–Brunt work given in Equation (25). The subscript p on the force $\bar{F}_p$ and on the d'Alembert (or deformation) force $\bar{\mathscr{D}}_p$ emphasizes that $p \equiv -(\partial U/\partial\hat{V})_S$ rather than P(H, S) is involved in the definition given in Equation (85f).

If the L in the definition $\mathcal{L} \equiv \int L\,d^3(\Lambda)\,dt$ is replaced by

$$L' \equiv [W - W_R(\Lambda, t)] - [U - U_R(\Lambda, t)] - M\phi = L - W_R + U_R \tag{86}$$

where $W_R(\Lambda, t)$ and $U_R(\Lambda, t)$ are specified reference energies, then it can be shown that $\delta^{(1+2)}\mathcal{L}' \equiv \delta^{(1+2)} \int L'\,d^3(\Lambda)\,dt$ is identical to Equation (85) except that $\bar{L}$ in the surface contribution given in Equation (85b) is replaced by $\bar{L}'$.

The terminal and boundary conditions to be imposed on the trial functions used in the action integral $\mathcal{L}$ are the same ones given in Equations (52) and (54) of Paper I for the kinetic action $\mathscr{W}$.

The expression for $\delta^{(1+2)}\mathcal{L}$ that is given in Equation (85) is valid for fluctuations about an arbitrarily chosen set of trial functions. If the standard terminal and boundary conditions are imposed on the trial functions, then only the integral given in Equation (85c) contains a first-order sensitivity to the fluctuations, so the necessary condition for

$\delta^{(1)}\tilde{\mathcal{L}} = 0$ is

$$\tilde{\mathscr{D}}_p = M\tilde{D}_t\tilde{V} + \frac{1}{\tilde{n}}\nabla\tilde{p} + M\nabla\tilde{\phi} = 0 \tag{87}$$

which is the equation of motion given in Equation (9).

The fact that the Euler–Lagrange equation for $\mathcal{L}$ agrees with the equation of motion for inviscid compressible flow proves that $\mathcal{L}$ is the action integral of a satisfactory variational principle, but an examination of $\delta^{(2)}\mathcal{L}$ given in Equation (85) shows that this variational principle is **not** simultaneously an energy principle. That is, the signs of the various contributions to $\delta^{(2)}\mathcal{L}$ are such that $\delta^{(2)}\mathcal{L}$ cannot be identified with any physically meaningful work or energy change. This is a consequence of the fact that the integrand (W – E) of Equation (81a) has no physical significance. The sum (W + E) is, of course, just the total instantaneous energy of the fluid, and if the Euler–Lagrange equation arising from $\delta^{(1)} \int (W + E)\,dt = 0$ were identical to the equation of motion given in Equation (9), $\int (W + E)\,dt$ would be the action integral of a satisfactory **variational energy** principle. However, this is **not** the case. The Euler–Lagrange equation that corresponds to $\delta^{(1)} \int (W + E)\,dt = 0$ has a force term with the wrong sign. Thus $\int (W - E)\,dt$ has the desired first variation but a physically meaningless second variation, whereas the reverse is true of $\int (W + E)\,dt$.

It will be shown in the next section that both the first and second variations of the action integral $\mathscr{A} \equiv \int (W + A)\,dt$ have the desired behavior, so $\mathscr{A}$ is the basis of a **variational energy** principle. In fact, $\mathscr{A}/(t_F - t_I)$ can be interpreted as the time-average of the total free energy of the system, and as such can be regarded as the appropriate thermodynamic potential function (or, more exactly, functional) of the total fluid system, in the sense that the total time-average free energy strives toward a minimum, and its departure

from this minimum is a measure of the departure of the system from equilibrium flow, i.e. flow that obeys the equations of motion.

Before demonstrating this, however, a few observations will be made regarding how the indefiniteness of the sign of $\delta^{(2)}\mathcal{L}$ impairs the utility of $\mathcal{L}$ as the basis for a direct (i.e. trial-and-error) solution of a flow problem. The integrand of Equation (85d) is the difference of two positive-definite quantities. Starting with the extremal set of trial functions $\widetilde{X}$ or $\widetilde{\Lambda}^A$, whether a change in the functional form of the trial functions will cause $\mathcal{L}$ to increase or decrease depends on which of the terms in Equation (85d) is more affected by the change. Thus the extremum is a saddle-point in parameter space, and the properties of this saddle surface are artifacts of the way the trial functions are parameterized rather than of the physical properties of the extremal flow. In particular, even if the extremal flow is physically stable, the extremum is still a saddle-point. This means that any attempt to solve a problem by making iterative adjustments in the parameters of the trial functions always in the direction of decreasing numerical value of $\mathcal{L}$ is almost certainly doomed to failure. These difficulties are compounded by the integral given in Equation (85e). For example, if a flow is physically stable both with respect to the second derivative of wind shear and with respect to buoyancy, then the integrand of Equation (85e), like that of Equation (85d), is the difference of two positive-definite quantities.

These considerations do not imply that the irreducible form of Hamilton's Principle is entirely useless for finding numerical solutions. Any solution scheme that is based solely on the vanishing of the first variation at the extremum will be insensitive to the unpredictability of the sign of the second variation. Such a scheme is in fact in common use: It consists of using Hamilton's Principle effectively to convert the equations of motion from partial differential equations into a system of algebraic equations. This is done by expressing

the trial functions as series expansions, the coefficients of which are the parameters of the variational problem. The condition that the first variation vanish becomes the condition that the first derivative of the action integral with respect to each parameter vanish, and this leads to the desired system of algebraic equations.

## VII. FREE-ENERGY FORM OF HAMILTON'S PRINCIPLE

### A. First and Second Variations of the Total Free Action

It was indicated at the end of the previous section that the action integral

$$\mathscr{A} \equiv \int_{t_I}^{t_F} (W + A)\, dt \tag{88a}$$

leads to a satisfactory variational energy principle. This will now be verified by a direct calculation of $\delta^{(1+2)}\mathscr{A}$. For the reasons discussed in Section III A of Paper I, this was carried out in a Cartesian inertial frame. When $\mathscr{A}$ is applied to a direct numerical solution of a flow problem, however, this can be carried out either in the convected frame or in an inertial frame.

In the convected frame $\mathscr{A}$ has the form

$$\mathscr{A} = \int_{(N,\,\Delta t)} [W + \hat{V}P(H, S) - M\phi(X, t) - H(\Lambda, t)]\, d^3(\Lambda)\, dt \tag{88b}$$

where the trial functions are $X(\Lambda, t)$ and $H(\Lambda, t)$; $W$ is the molar kinetic energy given by $W = \tfrac{1}{2}M(\partial_t X)_\Lambda \cdot (\partial_t X)_\Lambda$; $\hat{V} = J^X_\Lambda$ is the molar volume; $P(H, S)$ is the known pressure function; and $S(\Lambda, t)$ and $\phi(X, t)$ are given functions. $S(\Lambda, t)$ has no variation, but $\phi[X(\Lambda, t); t]$ does have a variation because its argument function $X(\Lambda, t)$ varies.

In a Cartesian inertial frame, $\mathscr{A}$ has the form

$$\mathscr{A} = \int_{(V,\,\Delta t)} [nW + P(H, S) - nM\phi(\boldsymbol{x}, t) - nH(\Lambda, t)]\, d^3(x)\, dt \tag{88c}$$

where now the trial functions are $\Lambda^A(\boldsymbol{x}, t)$, $(A = 1, 2, 3)$, and $H(\Lambda, t) = H[\Lambda^A(\boldsymbol{x}, t); t]$. The mole density is $n = J^\Lambda_x$, and $W$ is now given by Equations (81f, g). Since $\phi(\boldsymbol{x}, t)$ is a given function, it has no variation. Although $S(\Lambda, t)$ is a given function, it does have a

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variation because of its argument functions $\Lambda^A(\boldsymbol{x}, t)$, which is given in Equation (4). The molar entropy H varies both because of the variation of $\Lambda^A(\boldsymbol{x}, t)$, and also because of the variation of the functional dependence of $H(\Lambda, t)$. The total variation of H is given in Equation (69b). The pressure function P(H, S) is known, either as an empirical thermodynamic state function as illustrated in Equation (51) for the case of a perfect gas, or as an expansion of the type illustrated in Equation (57).

The expression for

$$\delta^{(1+2)}\mathscr{A} = \delta^{(1+2)}\int_{t_I}^{t_F}(W + A)\,dt = \delta^{(1+2)}\mathscr{W} + \int_{t_I}^{t_F}\delta^{(1+2)}A\,dt \quad (89a)$$

follows from Equations (70) and (84), and can be put into the following form:

$$\delta^{(1+2)}\mathscr{A} = [\delta^{(1+2)}\mathscr{W}]_T + [\delta^{(1+2)}\mathscr{A}]_S + \sum_{N=1}^{4}[\delta^{(1+2)}\mathscr{A}]_V^{(N)} \quad (89b)$$

where $[\delta^{(1+2)}\mathscr{W}]_T$ is given by Equation (84b) and

$$[\delta^{(1+2)}\mathscr{A}]_S = -\int_{(\mathscr{S},\Delta t)}\Big[(\bar{W} - \bar{H} - M\bar{\phi}) - \tfrac{1}{2}\delta X\cdot\nabla(\bar{W} - \bar{H} - M\bar{\phi}) + \bar{D}_t(M\bar{V}\cdot\delta X) - \tfrac{1}{2}\bar{\mathscr{D}}_P\cdot\delta X + \frac{\bar{N}}{\bar{n}}\delta_H H\Big]\delta^{(1+2)}n\cdot d\mathscr{S}dt\,; \quad (89c)$$

$$[\delta^{(1+2)}\mathscr{A}]_V^{(1)} = -\int_{(V,\Delta t)}[\bar{\mathscr{D}}_P\cdot\delta^{(1+2)}n + (\bar{n} - \bar{N})\,\delta_H H]\,d^3(x)\,dt\,; \quad (89d)$$

$$[\delta^{(2)}\mathscr{A}]_V^{(2)} = \int_{(V,\Delta t)}\Big[\tfrac{1}{2}\bar{n}M(\bar{D}_t\delta X)\cdot(\bar{D}_t\delta X) + \frac{1}{2\bar{\beta}}(\bar{N}\delta_H H + \bar{\beta}\nabla\cdot\delta X)^2\Big]\,d^3(x)\,dt\,; \quad (89e)$$

$$[\delta^{(2)}\mathscr{A}]_V^{(3)} = \int_{(V,\Delta t)}[\delta_X^{(2)}W + (\delta^{(2)}A)_S]\,\bar{n}\,d^3(x)\,dt\,; \quad (89f)$$

$$[\delta^{(2)}\mathscr{A}]_V^{(4)} = \int_{t_I}^{t_F} [\delta^{(2)}A]_V^{(5)}\, dt = -\int_{t_I}^{t_F} \delta_X^{(2)}Q\, dt\,; \tag{89g}$$

where

$$\bar{\mathscr{D}}_P \equiv M\bar{D}_t\bar{V} - \bar{F}_P = M\bar{D}_t\bar{V} + \frac{1}{\bar{n}}\nabla\bar{P} + M\nabla\bar{\phi}\,; \tag{89h}$$

$\bar{N}$ and $\bar{\beta}$ are defined in Equations (70i and j); $\delta_X^{(2)}W$ is defined in Equation (84f); $(\delta^{(2)}A)_S$ is the generalization of the Väisälä–Brunt work that is given in Equations (25 and (72e); $[\delta^{(2)}A]_V^{(5)}$ is given in Equation (70g); and $\delta_X^{(2)}Q$ is the second-order increase in heat or unavailable energy that results from substitution of Equation (42b) into Equation (44).

When the standard terminal and boundary conditions given in Equations (52) and (54) of Paper I are imposed, $[\delta^{(1+2)}\mathscr{W}]_T = [\delta^{(1+2)}\mathscr{A}]_S = 0$. Since $[\delta^{(1+2)}\mathscr{A}]_V^{(1)}$ given in Equation (89d) is the only surviving contribution to the variation that has a first-order sensitivity, the necessary conditions for $\delta^{(1)}\tilde{\mathscr{A}} = 0$ are

$$\tilde{\mathscr{D}}_P \equiv M\tilde{D}_t\tilde{V} + \frac{1}{\tilde{n}}\nabla\tilde{p} + M\nabla\tilde{\phi} = 0; \tag{90a}$$

$$\tilde{n} = \tilde{N} \text{ or } \tilde{J}_x^{\Lambda} = \widetilde{\left(\frac{\partial P}{\partial H}\right)_S}\,. \tag{90b}$$

The second condition implies that $\tilde{P} = \tilde{p}$, and this fact has been used in writing Equation (90a). These are the equations of motion that were stated in Equations (9) and (34). This agreement of the Euler–Lagrange equations of $\mathscr{A}$ with the known equations of motion of the fluid demonstrates that $\mathscr{A}$ is the action integral of a valid variational principle. The fact that $\mathscr{A}$ is also the basis of a valid energy principle follows from the demonstration given in Section V that A is the total free energy of a static atmosphere. Thus W + A is obviously the total free energy of a moving atmosphere, and $\mathscr{A}$ is essentially just the time-average of this total free energy.

It was pointed out in Section VI A of Paper I that, for any functional $\mathscr{A}$ that can be interpreted as the total time-average free-energy of the system, the condition

$$\delta^{(2)}\widetilde{\mathscr{A}} > 0 \tag{91}$$

is sufficient (but not necessary) for stability if the comparison class is limited to trial functions that satisfy a single set of imposed terminal and boundary conditions. Referring to the expressions given in Equation (89), it is evident in view of the Second-Law condition stated in Equation (44) that the only second-order term that has any chance of becoming negative is $[\delta^{(2)}\mathscr{A}]_V^{(3)}$. When use is made of Equations (25) and (84f), the resultant sufficient criterion for stability is

$$\begin{aligned} &\tfrac{1}{2}M\delta X\delta X:[\nabla(\widetilde{D}_t\widetilde{V}) - (\nabla\nabla\widetilde{V}) \cdot \widetilde{V}] \\ &\qquad + \tfrac{1}{2}\widetilde{n}[(\delta X \cdot \nabla \ell n\, \widetilde{n})(\delta X \cdot \nabla\widetilde{p}) - \widetilde{\beta}(\nabla \cdot \delta X)^2] > 0 . \end{aligned} \tag{92}$$

It must be emphasized that this criterion is valid only for a **restricted ensemble** of trial functions that satisfies a single specification of the standard terminal and boundary conditions. A special case of an **extended ensemble** will be discussed in subsection D below. Moreover, it must be recalled that this criterion refers to the onset of **internal instability** rather than **laminar instability**. (See Sections IV D and VI A of Paper I for a discussion of the distinction between these two types of instability.) In the commonly applied Boussinesq approximation, $\nabla \cdot \delta X = 0$ and the last term in Equation (92) drops out. If, in addition, the fluid has no density stratification, then $\nabla\widetilde{n} = 0$ and only the terms involving V remain. This is the form of the criterion that was applied in Section VI B of Paper I.

Finally, it should be noted that if W and H are referred to the reference energies $W_R(\Lambda, t)$ and $H_R(\Lambda, t)$ (both specified functions of $\Lambda^A$ and t) by replacing W and H in Equation (88) with $W' \equiv W - W_R$ and $H' \equiv H - H_R$, then the only change that occurs in Equation (89) is that in the surface term $[\delta^{(1+2)}\mathscr{A}]_S$ given in Equation (89c) $\overline{W}$ and

$\bar{H}$ are replaced by $\bar{W}'$ and $\bar{H}'$. If the standard boundary conditions are imposed, this surface integral vanishes in any case. This means that the inclusion of the specified reference levels $W_R(\Lambda, t)$ and $H_R(\Lambda, t)$ causes no change in either the Euler–Lagrange equations given in Equation (90), or in the stability criterion given in Equation (92). It was pointed out in Section VII of Paper I that the use of reference energies often provides a convenient way of avoiding a divergent action integral.

**B. Open Systems and Free Boundaries**

The surface integral $[\delta^{(1+2)}\mathscr{A}]_S$ given in Equation (89c) represents the decrease in $\mathscr{A}$ that results from transport of matter across the bounding surface $\mathscr{S}$. Thus, if the standard boundary conditions are not imposed and $\delta \mathbf{n} \cdot d\mathscr{S} \neq 0$ on $\mathscr{S}$, Equation (89c) gives the change in $\mathscr{A}$ that results from mass loss in an **open system** that is characterized by a fixed total volume V but a fluctuating total mole number N. If reference energies $W_R(\Lambda, t)$ and $E_R(\Lambda, t)$ for the kinetic energy W and the total static energy $E = U + M\phi$ are included, the surface term has the following form to first-order accuracy:

$$[\delta^{(1)}\mathscr{A}']_S = -\int_{(\mathscr{S}, \Delta t)} [(\bar{W} - \bar{W}_R) - (\bar{H} + M\bar{\phi} - \bar{E}_R)]\, \delta^{(1)}\mathbf{n} \cdot d\mathscr{S} dt. \quad (93)$$

This shows that if there is equipartition between the relative kinetic energy and relative static energy on the bounding surface, then the first-order surface contribution to the variation vanishes, i.e.

$$[\delta^{(1)}\mathscr{A}']_S = 0 \text{ if } (\bar{W} - \bar{W}_R) = (\bar{H} + M\bar{\phi} - \bar{E}_R) \text{ on } \mathscr{S}. \quad (94)$$

This kind of equipartition is characteristic of wave motion. In the case of such a problem, rather than impose the standard boundary condition $\delta \mathbf{X} \cdot d\mathscr{S} = 0$, it would often be more convenient or more realistic to leave X (or $\Lambda^A$) unconstrained on $\mathscr{S}$ and impose instead the equipartition requirement given in Equation (94). Because this makes $[\delta^{(1)}\mathscr{A}']_S = 0$,

the fulfillment of the Euler–Lagrange equations would still be a necessary condition for $\delta^{(1)}\mathscr{A}' = 0$. The imposition of the equipartition constraint on $\mathscr{S}$ is not sufficient to make the second-order surface contribution to the variation vanish. This non-vanishing second-order contribution can be given a meaningful physical interpretation, but it will in any case usually be overwhelmed by the second-order volume contribution to the variation.

A **free-boundary** problem is characterized by a fluctuating total volume V but a fixed total mole number N. In this case it is necessary to add a correction to Equation (93) in order to take $\delta V$ into account. If $\mathscr{A}'$ is written in the form

$$\mathscr{A}' = \int_{(V,\,\Delta t)} n\text{Ł}'\, d^3(x)\, dt \quad \text{where} \quad \text{Ł}' \equiv (W - W_R) - (U + M\phi - E_R), \tag{95a}$$

it is evident that the correction that must be added to Equation (93) is

$$[\delta_V^{(1)}\mathscr{A}']_S = \int_{\Delta t} dt \left[\int_{\mathscr{S}} \overline{n\text{Ł}'}\, \delta V\right] = \int_{\Delta t} dt \left[\int_{\mathscr{S}} \overline{n\text{Ł}'}\, \delta \mathbf{X} \cdot d\mathscr{S}\right]. \tag{95b}$$

Adding this correction to Equation (93) gives the first-order surface contribution to $\delta\mathscr{A}'$ at a free surface:

$$[\delta^{(1)}\mathscr{A}']_{FS} = \int_{(\mathscr{S},\,\Delta t)} \overline{P}\,\delta \mathbf{X} \cdot d\mathscr{S} dt = \int_{\Delta t} dt \left[\int_{\mathscr{S}} \overline{P}\,\delta V\right]. \tag{96}$$

This shows that $[\delta^{(1)}\mathscr{A}]_{FS}$ is just the time integral of the work that the system performs on its surroundings by virtue of changing its volume. This is the obvious generalization of the expression $\delta_V A = P\delta\hat{V}$ that was introduced at the beginning of Section III in connection with the virtual work performed by a one-mole sample of fluid.

Equation (96) does not take into account the work performed by the constant-pressure volume reservoir with which the system is in contact at the surface $\mathscr{S}$. If the

pressure of this reservoir is $p_0$, the expression for the total work performed by the system and the reservoir is

$$[\delta^{(1)}\mathscr{A}'']_{FS} = \int_{(\mathscr{S}, \Delta t)} (\bar{P} - p_0)\, \delta \mathbf{X} \cdot d\boldsymbol{\mathscr{S}} dt . \tag{97}$$

But this is just the first-order surface contribution to the variation of an action integral $\mathscr{A}''$ of the form

$$\mathscr{A}'' = \int_{(V, \Delta t)} [n\mathfrak{L}' - p_0(\boldsymbol{x}, t)]\, d^3(x)\, dt \tag{98a}$$

$$= \int_{(V, \Delta t)} \{n[W - W_R(\Lambda, t)] + [P(H, S) - p_0(\boldsymbol{x}, t)] - [H + M\phi - E_R(\Lambda, t)]\}\, d^3(x)\, dt \tag{98b}$$

where $p_0(\boldsymbol{x}, t)$ is a specified function of the inertial coordinates (and time). Obviously, in the inertial frame $\delta p_0 \equiv 0$ and its contribution to the total variation enters only in connection with the change in volume of the system at the free boundary. Thus $p_0(\boldsymbol{x}, t)$ is just a form of reference pressure, but unlike the other reference energies $W_R(\Lambda, t)$ and $E_R(\Lambda, t)$ which must be specified as functions of the Lagrange parameters $\Lambda^A$, $p_0$ must be a specified function of the inertial coordinates.

When $p_0$ is subtracted from the molar Lagrangian $\mathfrak{L}' = W' - (U + M\phi - E_R)$, it becomes $\mathfrak{L}'' = W' - [(U + p_0\hat{V}) + M\phi - E_R]$. That is, putting the system in contact with a volume reservoir with pressure $p_0$ requires the replacement of $U$ by $U + p_0\hat{V}$. This is just the generalization of the familiar transition from internal energy to enthalpy as the appropriate thermodynamic potential when contact with a constant-pressure reservoir is admitted. The important generalization is that the reservoir pressure $p_0$ may be an arbitrary (but specified) space–time function. For example, in the case of the evolution of a convection cell embedded in a surrounding atmosphere whose pressure field $p_0(\boldsymbol{x}, t)$ is a known

space–time function, the surrounding atmosphere serves as a volume reservoir for the convection cell.

All of these considerations hold for the irreducible form of Hamilton's Principle that was discussed in Section VI, the only difference being that $\mathcal{U} \equiv H - \hat{V}P$ is replaced by $U(\hat{V}, S)$. As a practical matter, however, this difference is very important. The reason is that, because in the free–energy form of Hamilton's Principle P(H, S) is an easily manipulated function, the condition $P = p_o$ on $\mathscr{S}$ is much easier to impose than the condition $p \equiv -(\partial U/\partial \hat{V})_S = p_o$ on $\mathscr{S}$. In the case of problems in static elasticity, Castigliano's Principle has the analogous advantage over Dirichlet's Principle.

A free–boundary problem is easiest to treat in the convected frame in which $\mathscr{A}''$ has the form

$$\mathscr{A}'' = \int_{(N,\,\Delta t)} \left\{ [\tfrac{1}{2}M(\partial_t X)_\Lambda \cdot (\partial_t X)_\Lambda - W_R] + [P(H,S) - p_o(X,t)] - [H + M\phi(X,t) - E_R] \right\} d^3(\Lambda)\, dt . \tag{98c}$$

The free boundary can be made to coincide with one of the $\Lambda^A$–surfaces. If $\Lambda^A_{\mathscr{S}}$ represents the numerical value of this coordinate, then the free boundary condition is

$$P[H(\Lambda^A_{\mathscr{S}});\ S(\Lambda^A_{\mathscr{S}})] = p_o[X(\Lambda^A_{\mathscr{S}})] \tag{99}$$

where for simplicity the time–dependence has not been indicated. Usually, it should be a simple matter to parameterize the trial functions $H(\Lambda)$ and $X(\Lambda)$ so that this condition will be satisfied. If this is not so easy, an alternative procedure can be applied: $\mathscr{A}''$ can be minimized without imposing the constraint of Equation (99). In this case, the extremum trial functions represent the best possible (within the limitations of the parameterization employed) **simultaneous solution** of both Equation (99) and the equations of motion given in Equation (90). This procedure corresponds to the fact that, even when the free–boundary condition $P = p_o$ on $\mathscr{S}$ is not satisfied, $\delta\mathscr{A}''$ is nevertheless equal to the change

in (time-average) free energy of the **total** system consisting of the system under study and the volume reservoir with which it interacts.

### C. Incompressible Limit

It was remarked following Equation (57) that one way to eliminate the explicit involvement of S in the formalism is to let the reference quantities in Equations (55-57) (designated by subscript o) be specified functions of $(\Lambda^A, t)$. If this is done in such a way that $S - S_o = 0$, the entropy dependence has effectively been absorbed into the remaining reference quantities and Equation (57), for example, becomes

$$P = p_o + n_o(H - H_o) + \tfrac{1}{2}\left(\frac{n^2}{\beta}\right)_o (H - H_o)^2 . \tag{100}$$

Incompressibility corresponds to the limit $\beta_o = n_o MC_o^2 \to \infty$. Passing to this limit, Equation (100) becomes

$$P = n_o H - u_o \text{ where } u_o = n_o H_o - p_o . \tag{101}$$

$n_o$, $H_o$, and $p_o$ may all be functions of $\Lambda^A$, but if it is further required that $\nabla u_o = 0$, then $u_o$ is a numerical constant or at most a function only of t. This requirement provides a way of decoupling internal thermal energy from kinetic or gravitational energy. $n_o = n_o(\Lambda)$ is a constant of motion as in the Boussinesq approximation. Because of this, the total volume $V = \int \hat{V} d^3(\Lambda)$ occupied by the fluid must be constant, and since $u_o$ is at most a function only of t, $\delta \int u_o \hat{V} d^3(\Lambda) = 0$. Substituting Equation (101) into Equation (88b) and dropping $(-u_o \hat{V})$ from the integrand, the action integral becomes

$$\mathscr{A} = \int_{(N,\,\Delta t)} [\tfrac{1}{2}M(\partial_t X)_\Lambda \cdot (\partial_t X)_\Lambda - M\phi(X, t) + (\hat{V} n_o - 1)\, H(\Lambda, t)]\, d^3(\Lambda)\, dt \tag{102}$$

whose Euler-Lagrange equations are

$$(\partial_t^2 \tilde{X})_\Lambda \equiv \tilde{D}_t \tilde{V} = -\nabla\tilde{\phi}\,; \quad \tilde{n} = n_o(\Lambda)\,; \tag{103a, b}$$

which are the equations for incompressible flow in a gravitational field. For non-extremal flows $n \equiv 1/\hat{V} \neq n_0(\Lambda)$, so the class of virtual flows admits compressibility. Thus the action integral of Equation (102) is best pictured as describing a compressible fluid that is flowing at such low Mach numbers that its macroscopic behavior is that of an incompressible fluid, but on a microscopic level turbulent density fluctuations are possible. The equation $\tilde{n} = n_0$ is the condition that must be satisfied if $\mathscr{A}$ is to be insensitive to fluctuations in H. From this perspective, $H(\Lambda, t)$ is a Lagrange multiplier that arises from the imposed constraint $\hat{V}n_0 = 1$. The variational principle based on Equation (102) with $H(\Lambda, t)$ interpreted as a Lagrange multiplier is very well known[20] and was formulated by Lagrange.[21] It is, in fact, the very first variational principle for a continuum.

A more extreme incompressible limit results from transforming Equation (102) to an inertial frame and parameterizing the $\Lambda^A(\boldsymbol{x}, t)$ in such a way that $\delta n \equiv \delta J_x^\Lambda = 0$ identically. This corresponds to a really incompressible fluid, not merely a compressible fluid with vanishing Mach number. It can be shown that in this case only the kinetic energy term has a non-vanishing variation, so this variational principle is just the one considered in Section V of Paper I.

## D. Buoyancy Stability of a Shearing Wind

It was noted following the stability criterion that was stated in Equation (92) that this criterion is valid only for the **restricted ensemble** of trial functions that satisfy a single specification of the standard boundary and terminal conditions. When these conditions are relaxed an **extended ensemble** results for which the terminal and surface contributions in Equation (89) may no longer vanish. Such a case was discussed in Section VI C of Paper I. The extended ensemble consisted of all dynamically acceptable horizontal winds for which the **total** mass flux or momentum equalled a specified value. It was shown that

if two blobs of fluid separated by a vertical distance $\delta z$ exchange positions and in so doing exchange momentum with their new surroundings, a reduction in the total kinetic action will result. The calculation was carried out for a linear wind profile, i.e. a constant shear $(d\tilde{V}/dz)$, and was normalized so that each blob contained one-half mole of fluid. The resulting change in the time-average kinetic action which was given in Equation (79) of Paper I is

$$\delta^{(2)}\tilde{\mathscr{W}}/\Delta t = -(1/8)\, M(d\tilde{V}/dz)^2\, (\delta z)^2 . \tag{104}$$

This change in time-average action must be added to the time-average change of $[\delta^{(2)}\mathscr{A}]_V^{(3)}$ given in Equation (89f) (which gave rise to the criterion given in Equation (92)). For a constant wind shear $d^2\tilde{V}/dz^2 = 0$ and $\bar{D}_t\tilde{V} = 0$, so for a Boussinesq exchange of two ½-mole blobs separated by a vertical distance $\delta z$ in an atmosphere in hydrostatic equilibrium so that $\nabla\tilde{p} = -Mg\tilde{n}\,e_z$,

$$[\delta^{(2)}\mathscr{A}]_V^{(3)}/\Delta t = -\tfrac{1}{2}Mg\,\frac{d\,\ell n\,\tilde{n}}{dz}\,(\delta z)^2 . \tag{105}$$

The total change in the time-average action (or free energy) is the sum of Equations (104) and (105), and the sufficient condition for stability is that this sum be positive:

$$\tfrac{1}{2}M\left[\left(-g\,\frac{d\,\ell n\,\tilde{n}}{dz}\right) - (1/4)\,(d\tilde{V}/dz)^2\right](\delta z)^2 > 0 \tag{106a}$$

or

$$\mathscr{R}i \equiv \frac{(-g\,d\,\ell n\,\tilde{n}/dz)}{(d\tilde{V}/dz)^2} > 1/4 \tag{106b}$$

where $\mathscr{R}i$ is the Richardson number defined on the Boussinesq static stability measure $(-g\,d\,\ell n\,\tilde{n}/dz)$. If, instead of the Boussinesq condition $\nabla\cdot\delta X = 0$, the quasi-static condition $\nabla\cdot\delta X = -\delta X\cdot\nabla\tilde{p}/\tilde{\beta}$ had been used in Equation (89f), the numerator in the Richardson number would have been the Väisälä-Brunt stability measure $g[-(d\,\ell n\,\tilde{n}/dz) - g/\tilde{C}^2]$. The sufficient condition stated in Equation (106b) is just the well-known condition

of Miles[4] and Howard[5] that was derived by entirely different means within the context of a normal-mode analysis.

## E. The Thermodynamic Inequality

By subtracting Equation (85) from Equation (89) it is found that in the neighborhood of an extremum

$$\delta^{(1+2)}\widetilde{\mathscr{A}} - \delta^{(1+2)}\widetilde{\mathscr{L}} > 0 \tag{107}$$

if the flow is stable so that $\delta^{(2)}\widetilde{A}_{VB} > 0$ and $\delta^{(2)}\widetilde{A} > 0$, and if $\delta_H H = 0$ on $\mathscr{S}$, and the fluctuations satisfy the Second-Law requirement $\int \delta^{(2)}\Omega \, dt \leqslant 0$. This is true even if the standard terminal and boundary conditions are not imposed. Because $\widetilde{\mathscr{A}} = \widetilde{\mathscr{L}}$, it follows that in the neighborhood of an extremum

$$\langle W + A \rangle_t \geqslant \langle W - E \rangle_t , \tag{108}$$

where $\langle \quad \rangle_t$ designates the time average. This inequality can be useful in numerical applications of the free-energy form of Hamilton's Principle to estimate the error that still remains in an approximate solution that was obtained by minimizing $\langle W + A \rangle_t$ for a certain choice of parameterization. This best answer can be inserted into the irreducible form of Hamilton's Principle in order to calculate the right side of Equation (108). The difference between the two sides of this inequality is then a measure of the error of the approximate solution. Obviously this error measure is not sensitive to errors in the kinetic energy. Subtracting $\langle W \rangle_t$ from both sides of Equation (108) yields

$$\langle A \rangle_t \geqslant -\langle E \rangle_t \tag{109}$$

which is subject to the same conditions that were stated following Equation (107). The two sides of Equation (109) are related by a Friedrichs transformation[2] (elimination of the extensive variable n in favor of the intensive variable H by means of a Legendre transformation), and the inequality of Equation (109) is the basis of the minimax formulation that is the characteristic result of a Friedrichs transformation. The thermodynamic meaning

of this inequality follows from the observation that because $A = -\int (\mathcal{U} + M\phi)\, dN$ and $E = \int (U + M\phi)\, dN$, the common gravitational energy can be subtracted from both sides of Equation (109) yielding

$$\langle \mathcal{U} \rangle_t \leqslant \langle U \rangle_t \equiv \langle \tilde{\mathcal{U}} \rangle_t \tag{110}$$

which is the generalization to an extended time-dependent fluid system of the simple thermodynamic inequality $\mathcal{U}(H, \hat{V}, S) \leqslant U(\hat{V}, S)$ that was given in Equation (39).

The inequality of Equation (110) excludes both kinetic and gravitational energy. It will now be shown that when total time-average internal energy is defined in the only way that is permissible in the context of Special Relativity the relativistic version of Equation (110) is identical to

$$\langle W + A \rangle_t \geqslant \langle \tilde{W} + \tilde{A} \rangle_t \tag{111}$$

which follows from Equation (89) if the flow is physically stable and the Second-Law constraint given in Equation (44) is satisfied. That is, in a relativistic context, the statement that the total time-average internal free energy of a fluid system tends to a minimum is equivalent to the statement that the properly defined total time-average internal thermal energy $\langle \mathcal{U}_{REL} \rangle_t$ tends to a maximum. This may be regarded as the relativistic statement of the Second Law in the energy representation.

The demonstration results from writing

$$\langle W + A \rangle_t = \frac{1}{\Delta t} \int_{(N,\, \Delta t)} [\tfrac{1}{2} MV^2 - \mathcal{U} - M\phi]\, dN\, dt \tag{112}$$

in relativistic form or by following the converse procedure and showing that $\frac{1}{\Delta t} \int [\int \mathcal{U}_{REL}\, d\tau]\, dN$ is equivalent to Equation (112), where $d\tau = dt(1 - V^2/c^2)^{1/2}$ is the proper time interval and

$$\mathcal{U}_{REL} = M_o c^2 + M_o(\phi - \phi_o) + \mathcal{U} \tag{113}$$

is the relativistic molar internal energy. (The same definition also applies to $U_{REL}$ and U.) $M_0c^2$ is the molar rest-mass at the point where the gravitational potential equals the reference value $\phi_0$ and $M_0(\phi - \phi_0)/c^2$ is the mass increase attributable to the increase in gravitational potential. (This is the scalar or Nordström theory of gravitation which is consistent with Special Relativity, but is not adequate to explain some of the subtler gravitational effects for which General Relativity is necessary.) Because the internal thermal energy is the average internal kinetic energy of molecular motion, the rest-mass and the gravitational contribution to the mass are inseparable from the internal thermal energy in a relativistic context. Moreover, because the average internal kinetic energy must be defined in the local rest-frame of the gas, the only acceptable relativistic generalization of $\mathcal{U}dt$ is

$$\begin{aligned} \mathcal{U}_{REL}\, d\tau &= [M_0c^2 + M_0(\phi - \phi_0) + \mathcal{U}]\,(1 - V^2/c^2)^{1/2}\, dt \\ &= [M_0c^2 + M_0(\phi - \phi_0) + \mathcal{U} - \tfrac{1}{2}M_0V^2 - \tfrac{1}{2}M_0V^2(\phi - \phi_0)/c^2 \\ &\qquad - \tfrac{1}{2}M_0V^2(\mathcal{U}/M_0c^2) + O^4(V/c)]\, dt \\ &\approx [M_0c^2 + M_0(\phi - \phi_0) + \mathcal{U} - \tfrac{1}{2}M_0V^2]\, dt\,. \end{aligned} \tag{114}$$

Except for the term $M_0c^2(1 - \phi_0/c^2)\,dt$ whose inclusion in the integral of Equation (112) makes no difference as far as variations are concerned, the right side of Equation (114) is equal to the negative of the integrand in Equation (112). Because Equation (114) also applies for the equilibrium configuration, it is evident that Equation (111) is equivalent to

$$\langle \mathcal{U}_{REL} \rangle_t \leqslant \langle \tilde{\mathcal{U}}_{REL} \rangle_t \text{ where } \langle \mathcal{U}_{REL} \rangle_t \equiv \frac{1}{\Delta t} \int_N dN \left[ \int_{t_I}^{t_F} \mathcal{U}_{REL}\, d\tau \right]. \tag{115a, b}$$

Moreover,

$$\langle W + A \rangle_t = NM_0c^2(1 - \phi_0/c^2) - \langle \mathcal{U}_{REL} \rangle_t\,, \tag{115c}$$

which is the generalization of the relation $A = -\mathcal{U}$ that was used in Section III.

In the case of a cold gas moving in the absence of a gravitational field, $U_{REL}$ reduces to $M_o c^2$, and Equation (115a) reduces to the relativistic way of saying that all the particles prefer to move in straight lines.

Equation (115a) is the relativistic thermodynamic inequality. It says that the total disordered heat energy, i.e. the kinetic energy of random internal motion as viewed in the local macroscopic rest-frame and summed over all the matter, strives toward a maximum. This obviously is one way to state the Second Law.

If the fluid system under consideration is "viewed from afar," the fluctuating trial functions $\Lambda^A(\mathbf{x}, t)$ and $H(\Lambda, t)$ could be identified with what thermodynamicists refer to as "internal degrees of freedom" (usually pictured as imaginary internal partitions). When these have assumed their preferred (i.e. equilibrium) values, the equilibrium thermodynamic energy can be described exclusively in terms of such things as total volume and total entropy that are insensitive to fluctuations in the internal degrees of freedom. The corresponding quantities in the case of the variational principle are the total mole number N (or total volume V in the case of an open system), the specified molar entropy $S(\Lambda, t)$, and the average particle velocity $\langle V \rangle_t \equiv (X_F - X_I)/\Delta t$ that is specified by the terminal conditions. $\langle \tilde{W} + \tilde{A} \rangle_t$ is a function of these specified quantities, which are non-denumerably infinite in number. If it were known as an analytical function for all possible values of these specified quantities, the resulting function would be the equilibrium thermodynamic potential function for the system. Even without having an explicit expression for this potential function, the expressions for the variation of the action integral that have been derived above can be used to determine how the equilibrium thermodynamic potential function of the system changes under differential changes in the specified quantities (such as $\langle V \rangle_t$) on which it depends. Such differential expressions can be used in turn in

connection with thermodynamic theorems such as the LeChatelier-Braun[22] principle to determine how changes in certain specified quantities will affect various secondary quantities that can be derived from the equilibrium potential function.

The relation between the non-equilibrium action integral (which has been called the "total time-average internal free energy") and the equilibrium action integral (which has been called the "equilibrium thermodynamic potential of the total system") can be very simply illustrated in the case of a homogeneous fluid by the inequality

$$\mathcal{U}(H, \hat{V}) \leqslant \mathcal{U}(\tilde{H}, \hat{V}) \equiv \tilde{U}(\hat{V}) \qquad (116)$$

which, except for the fact that the S-dependence has been suppressed for the sake of simplicity, is the thermodynamic inequality that was given in Equation (39). H is to be regarded as representative of the fluctuating "internal degrees of freedom" and $\hat{V}$ as representative of the specified constants of motion or average quantities that characterize the equilibrium state. The fact that $\mathcal{U}(H, \hat{V})$ has its maximum at equilibrium implies that

$$0 = \left[\frac{\partial \mathcal{U}}{\partial H}\right]_{H = \tilde{H}} = \left[\frac{\partial}{\partial H}(H - \hat{V}P)\right]_{H = \tilde{H}} = 1 - \hat{V}N(\tilde{H}) \qquad (117)$$

where $N \equiv (\partial P/\partial H)_S$. This relation can be solved to give $\tilde{H}$ as a function of $\hat{V}$ which can then be substituted into $\mathcal{U}(\tilde{H}, \hat{V})$ to give $\tilde{U}(\hat{V})$. This can be done for different values of $\hat{V}$, with the result that $\tilde{U}(\hat{V})$ can be pictured as the ridge-line that connects all of the maxima for different values of $\hat{V}$. This is illustrated in Figure 3A. The projection of the $\mathcal{U}(H, \hat{V})$ surface onto the $\mathcal{U} - \hat{V}$ plane is pictured in Figure 3B (the section curves shown in Figure 3A becoming straight vertical lines in Figure 3B). The fact that all of the virtual fluctuations fall below $\tilde{U}(\hat{V})$ in Figure 3B is reminiscent of Caratheodory's characterization[23] of the equilibrium state function as the boundary between allowed and forbidden regions of thermodynamic phase space (although he was referring to real spontaneous processes rather than to virtual fluctuations).

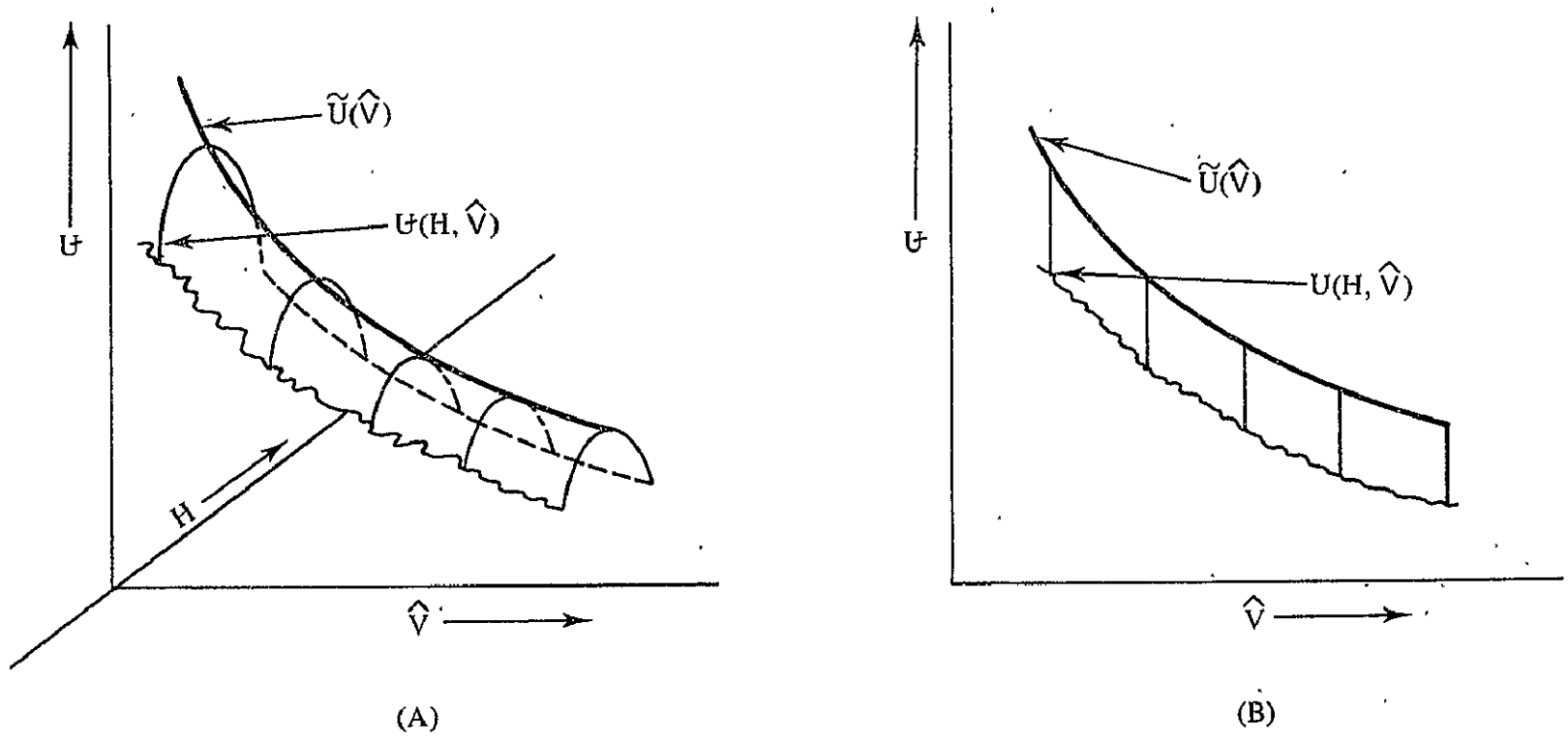


Figure 3. (A) Non-Equilibrium Internal Energy Surface $\mathcal{U}(H,\hat{V})$ and its Ridge-Line, the Equilibrium Internal Energy $\tilde{U}(\hat{V})$. (B) Projection of Figure A onto ($\mathcal{U}$ – $\hat{V}$)-Plane Showing $\tilde{U}(\hat{V})$ as Boundary of Region of Virtual Fluctuations.

It might seem remarkable that, knowing only the empirical equilibrium state function P(H, S), it has been possible to construct the higher-dimensionality non-equilibrium surface $\mathcal{U}(H, \hat{V}, S)$. In fact, however, the construction $\mathcal{U} \equiv H - \hat{V}P(H, S)$ is not unique. The function

$$\mathcal{U} \equiv H - \hat{V}P(H, S) - \tfrac{1}{2}K^2[\hat{V}N(H, S) - 1]^2 , \qquad (118a)$$

where K is any constant, would do just as well. In fact, if used in the variational principle, it would increase the convexity with respect to the $\delta X$ or $\delta \Lambda^A$ fluctuations, and thereby improve the convergence. The physical significance of the extra term becomes apparent from the fact that $P_{EXT}$, the pressure of the surrounding fluid in the immediate neighborhood of an expanding sample of fluid is given by

$$P_{EXT} \equiv -\frac{\partial \mathcal{U}}{\partial \hat{V}} = P(H, S) + K^2N(\hat{V}N - 1) \qquad (118b)$$

Since $P_{EXT} > P(H, S)$ if $\hat{V} > 1/N$, the excess over P(H, S) can be interpreted as the increase in external pressure that results from the "snowplow effect" produced in the fluid that is immediately outside a sample cell that has expanded beyond its equilibrium size. The magnitude of $K^2$ is some function of the ratio of the typical speed of this non-equilibrium expansion and the speed of sound in the fluid. Such an "internal Mach number" would characterize the violence of the fluctuations. The case $K^2 = 0$ that has been discussed in this paper corresponds to the limiting case of very slow (i.e. quasi-static) volume fluctuations. This is just the case for which the equilibrium expression P(H, S) gives a valid description of the external pressure $P_{EXT}$.

The free energy that corresponds to the simple example of Figure 3A is $A \equiv -\mathcal{U}$ so the corresponding figure for A would be given by reflecting the surface in the $H - \hat{V}$ plane. The equilibrium ridge line now becomes an equilibrium trough line, and the height of any point on the surface above the point of the trough line for the same $\hat{V}$ represents the

internal non-equilibrium free energy. The generalization of this to a fluid in motion is the difference between the two sides of Equation (111) which gives the time-average total free energy of the fluctuations or turbulence within the fluid.

The difference $\mathscr{A} - \tilde{\mathscr{A}}$ refers to the free energy of turbulence about equilibrium, which is of second order in the fluctuations $\delta X$ and $\delta_H H$. The difference $\mathscr{A} - \bar{\mathscr{A}}$, where $\bar{\mathscr{A}}$ refers to an arbitrary set of trial functions, has a first-order dependence on $\delta X$ and $\delta_H H$ which by Equation (89d) is given by

$$\delta^{(1)}\mathscr{A} = \int_{(V,\,\Delta t)} [(-\delta X \cdot \bar{\mathscr{D}}_P) - \delta_H Q]\, \bar{n}\, d^3(x)\, dt \tag{119}$$

where $\delta_H Q$ is given in Equation (42a). (It has been assumed that the standard terminal and boundary conditions have been imposed.) As explained in connection with Equation (43), the first-order integral of the heat term either vanishes or else can be interpreted as the heat transferred to a reservoir. The integral of $(-\delta X \cdot \bar{\mathscr{D}}_P)$ represents the total work done by the system under study on another system (real or imaginary) that is coupled to it in such a way that it introduces the molar force $\bar{\mathscr{D}}_P$ into the equation of motion. (Cf. Eq. (10a).) Thus Equation (119) represents the change in free energy of this new interacting system that is coupled to the fluid system under study through the imposed force $\bar{\mathscr{D}}_P$. To the extent that $\bar{\mathscr{D}}_P$ can be given real physical meaning, $\bar{\mathscr{A}}$ can be interpreted as an equilibrium free energy for a flow whose equation of motion includes $\bar{\mathscr{D}}_P$. If $\delta^{(2)}\bar{\mathscr{A}} > 0$, this equilibrium is stable.

When we start with some arbitrary set of trial functions and vary these by successive iterations always so as to decrease $\mathscr{A}$, we can give this process the interpretation that the system represented by $\mathscr{A}$ is doing work on another system coupled to it by the force $\mathscr{D}_P$. The work delivered, and hence the change in $\mathscr{A}$, is path-dependent, that is, it is different

for the different paths in parameter space that correspond to different iteration procedures. This fact is very important for the application of the free-energy form of Hamilton's Principle to numerical solutions.

## F. Direct Solution of a Flow Problem by Minimizing the Total Free Action

The basic idea is that if a suitable energy sink is available, the free energy of a system will tend to drop to a minimum. In the case of a box of gas, one could start with an arbitrary initial state and relax imaginary internal membranes that are coupled to a suitable energy sink so as to bring the appropriate total thermodynamic potential of the gas to a minimum, which yields the desired equilibrium state. The analogous process in the case of a compressible inviscid fluid is to start with some initial state (i.e. choice of trial functions) and move the membranes (Lagrange surfaces) described by them and simultaneously redistribute the enthalpy so as to bring the appropriate thermodynamic potential, which is $\mathscr{A}$, from its initial value to its minimum value, which then describes the desired equilibrium state. In the course of relaxing the internal membranes, energy is delivered from the system to an imaginary sink that is coupled to it through the force $\mathscr{D}_p$, which vanishes at equilibrium.

It must be emphasized at the outset that whether or not one indeed arrives at a minimum value of $\mathscr{A}$ by this process, or, if so, whether the minimum is the desired one (i.e. whether the equilibrium flow has the desired topological properties), depends critically on the starting point in parameter space (i.e. the initial choice of trial functions) and on the details of the iteration process which determine the particular downward (i.e. in the direction of decreasing $\mathscr{A}$) path in parameter space. For example, if the topology of the $\mathscr{A}$-surface in parameter space is such that there is a ridge between the valley containing the desired minimum and the starting point, then a downward path from the starting point will

not lead to the desired minimum. Either it will lead to a different minimum or, will plunge into the void ($\mathscr{A} \to -\infty$). Even if no ridge separates the goal from the starting point, the same thing can happen. For example, if the desired minimum is at the bottom of a crater that is surrounded by a ridge having a low lip or mountain pass at one point, then starting at a point on top of the ridge it is possible that one downward path (iteration procedure) will lead to the bottom of the crater as desired, whereas a different iteration procedure will produce a downward path that will pass through the lip and on into the void beyond.

It is obvious from these examples that unless one is able to start from a point well within the bowl containing the desired minimum, one must be prepared to make false starts. To avoid pursuing a hopeless course for too long, it is necessary to monitor some quantity that will indicate when the iteration procedure is heading in a nonsensical direction. For example, one could monitor a thermodynamic quantity that must be positive to have physical meaning. If this goes negative, the iteration can be stopped and a new starting point chosen. In low Mach-number flows, the density varies very little from its static value. A large and increasing difference from the static value would indicate a false start.

An alternative procedure is to start with a problem that differs by very little from one whose solution is known. In such a problem the starting point can be chosen very close to the desired solution. For example, if the problem is to find the flow past an object in a wind with strong shear when the flow for no shear is known, the shear can at first be made very small. When this problem is solved, it can be used as the starting point to solve the same problem with slightly stronger shear, and so on.

If it can be assumed that (by one means or another) the starting point has been placed within the bowl containing the desired equilibrium point at its bottom, then a straightforward steepest-descent iteration can be employed until the gradient of $\mathscr{A}$ (in parameter

space) becomes small. At this point the second-variation given in Equation (89) becomes comparable in magnitude with the first variation, and it is necessary to impose the Second-Law condition

$$\int_{\Delta t} \delta^{(2)}Q\, dt = \int_{(V,\Delta t)} (\delta^1 n)\,(\delta_H H - \delta_X \bar{P}/\bar{n})\, dV dt \leqslant 0 \qquad (120a)$$

or

$$\int_{(V,\Delta t)} \nabla \cdot (\bar{n}\delta X)\,(\delta_H H - \delta X \cdot \nabla\bar{P}/\bar{n})\, d^3(x)\, dt \geqslant 0 \qquad (120b)$$

which is obtained from Equations (44), (70g) and (15d). The reason that this condition must be imposed is that, although the functional $\mathscr{A}$ has been constructed to provide a reasonably faithful mathematical description of the fluctuations that occur in a turbulent fluid, it cannot by itself imitate the kind of correlation between independent fluctuations that is required by the Second Law. It was pointed out following Equation (44) that this correlation simply says that, on the average, when heat flows into a sample of fluid, the fluid must expand, and when heat leaves, the fluid must contract. The same interpretation applies to the correlation between $\delta^{(1)}n$ and $\delta_H H$ (for $\delta X \cdot \nabla\bar{P} = 0$). For $\delta_H H = 0$, the correlation between $\delta^{(1)}n = -\nabla \cdot (\bar{n}\delta X)$ and $\delta X \cdot \nabla\bar{P}/\bar{n}$ says that, on the average, when a sample is carried into a region of greater pressure, it must diminish in size.

In a direct solution, the condition stated in Equation (120) could be imposed by making a calculation of the integral in Equation (120b) for a proposed iterative step that has been shown to cause a decrease in $\mathscr{A}$. If the integral of Equation (120b) is not negative, the iterative step is accepted and a new step is then made and tested in the same way. If the integral of Equation (120b) is found to be negative, the iterative step is altered so as to satisfy the condition (and simultaneously decrease $\mathscr{A}$).

When the condition of Equation (120) is satisfied at every iterative step, then reference to Equation (89) shows that, if the flow is physically stable, then $\delta^{(2)}\mathscr{A} > 0$, which means that for the admitted class of iterations the equilibrium point is a **minimum** and not a saddle-point, and this fact guarantees that the procedure of successive decreases in $\mathscr{A}$ will indeed lead to the equilibrium point.

This fact illustrates the great advantage of the free-energy form of Hamilton's Principle over the irreducible form. Reference to Equation (85) shows that, even for physically stable flow, $\delta^{(2)}\mathcal{L}$ is indefinite in sign, and there is no simple way of restricting the class of iterations so that it will be positive-definite. Thus the equilibrium point is a very intricate saddle-point, and it becomes extremely difficult to devise an iterative procedure that will "home in on it."

It should be noted that the condition imposed in Equation (120) is so weak that in many problems it could be ignored altogether without causing trouble. The reason for this is that it involves an **integral** over the **products of independent fluctuations** that in most problems will have different signs in different regions so that the resultant integral will usually be very small. This is to be contrasted with the other terms in $\delta^{(2)}\mathscr{A}$ given in Equation (89). In these integrals there is no cancellation, so they are usually very much larger than the integral of Equation (120). Thus, for most problems, even if the Second-Law condition is violated, $\delta^{(2)}\mathscr{A}$ will still be positive and so the iterative procedure will "home in on" the equilibrium point without any problem. The fact that the condition of Equation (120) is an inequality rather than an equality means that, even in an analytical non-numerical application of the direct solution method, the condition can often be accommodated. Because it is not necessary that the integral have any particular value, but rather only a particular sign, after the trial functions have been parameterized, an analytical

calculation of the integral in Equation (120) can be made. If certain of the parameters are then found to violate the condition, they can either be suppressed (dropped from the parameterization scheme) or else limited in their ranges so that their variations will not violate the condition.

## VIII. CONCLUDING REMARKS

The total free action functional $\mathscr{A}[\Lambda^A(\boldsymbol{x}, t); H(\Lambda^A, t); S(\Lambda^A, t)]$ that was constructed in Section VII A is the generalization of the non-equilibrium potential function $[-\mathcal{U}(\hat{V}, H, S)]$ for a static homogeneous fluid. The functional $\mathscr{A}$, like the function $\mathcal{U}$, must satisfy the basic thermodynamic inequality that describes the fluctuations of a system about equilibrium. In the case of $\mathcal{U}$, it is an easy matter to construct a function $\mathcal{U}(\hat{V}, H, S)$ (cf. Eqs. (38) and (118a)) that will automatically satisfy this inequality. In the case of the functional $\mathscr{A}$, it does not suffice to give $\mathscr{A}(\Lambda^A, H, S)$ a suitable functional dependence because subtle correlations between the space-time dependence of the otherwise independent fluctuations of $\Lambda^A$ and H are involved in the thermodynamic inequality, and for this reason it is necessary to impose the very weak integral constraint stated in Equations (44) and (120). As far as numerical applications involving $\mathscr{A}$ are concerned, this constraint represents at worst an annoyance, and can in fact be ignored in a great many numerical applications.

It is interesting to note that in the expression for $\delta^{(2)}\mathscr{A}$ given in Equation (89), the term on which this constraint must be imposed (cf. Eqs. (70g) and (89g)) is not symmetric in the particle displacement $\delta X$, whereas all the other second-order terms in $\delta^{(2)}\mathscr{A}$ are symmetric in $\delta X$, and so correspond to a self-adjoint energy operator that represents the energy of small displacements from equilibrium. The non-symmetric term $-\int \delta_X^{(2)} \mathcal{Q}\, dt$ vanishes if the displacements are density-preserving or adiabatic.

As to the practical utility of the total free action $\mathscr{A}$, besides its use in a direct solution of flow problems, there are the other possibilities that were suggested at the end of Section VII E. Because the methodology of equilibrium thermodynamics has effectively been extended to fluid systems in arbitrary states of motion with the recognition that $\mathscr{A}$

is the appropriate equilibrium potential function for such a system, and that the surface and terminal integrals of Equation (89) are the generalizations of the Pfaffian forms on which the classical thermodynamic formalism is based, the possibility is opened of extending thermodynamic principles and methodology to the problems of fluid dynamics. The second-order expressions for $\delta^{(2)}\mathscr{A}$ should be especially useful in this regard. It was shown in Section VII D how a well-known stability criterion can be derived very directly from the expression for $\delta^{(2)}\mathscr{A}$. In practical applications in dynamic meteorology, for example, the functions $\Lambda^A(\mathbf{x}, t)$ would be parameterized in terms of parameters of direct significance representing such things as the diameter or height of a convection cell, the total strength of its updraft, etc. It would then be a simple matter to derive an expression for $\delta^{(2)}\mathscr{A}$ in terms of a bilinear form in the variations of these parameters. Such an expression not only provides a stability criterion in terms of non-local parameters that would be very difficult to derive by other means, but the second order terms in the expression supply the raw material necessary to apply the LeChâtelier-Braun Principle[22] with which to explore the effects of perturbations from equilibrium.

Aside from the practical utility of constructing the effective thermodynamic potential function that governs compressible inviscid flow, there is also the conceptual satisfaction of basing Hamilton's Principle on more fundamental principles. Far from being a mere mathematical artifice, the free-energy form of it is a thermodynamic potential. The irreducible form of it, however, remains in the artifice category. The identification of the free-energy form of Hamilton's Principle with a thermodynamic potential has opened the treatment of its second variation to an entirely new perspective, one that would be unattainable by mathematics alone because it involves an admixture of physics in the form of the Second Law. Moreover, this identification provides a physical significance to the fact that Hamilton's Principle involves terminal, rather than initial, conditions. (See Section IV D

of Paper I.) The awareness that such terminal conditions can have a physical significance quite distinct from initial conditions leads to the distinction between two very different classes of instability—the laminar and internal types of instability that were discussed in Section VI A of Paper I.

The treatment presented here is not unique. Allusions have been made to a more general treatment based on $u(n, \phi)$ and P(G, T) instead of $u(n, S)$ and P(H, S). Both of these treatments represent extensions of the energy representation of thermodynamics. It is reasonable to expect that a corresponding treatment would be possible in the context of the entropy representation. The action integral corresponding to $\mathscr{A}$ would then be the time integral of either the total entropy or else of one of the Massieu functions[24] derived from it. The formalism based on such an action integral should have a strong resemblance to the formalism of statistical mechanics, and in fact the treatment of extended ensembles (cf. Sections VI A and C of Paper I) in the context of such an action integral might be the basis of a statistical mechanics of continuum ensembles.

## APPENDIX: BRIEF LITERATURE SURVEY

### A.1 Various Approaches Employed

It is possible to identify five different main lines of approach in the history of attempts to construct variational principles for fluid flow. The first is in the spirit of Lagrange's principle[21] that was mentioned in Section VII C above. One starts with a known variational principle for particle motion (the Least Action Principle of Maupertuis and Euler in Lagrange's case) and then adapts it to the fluid case by using the method of Lagrange multipliers to add appropriate constraints.

The second approach is to apply Hamilton's Principle directly to a fluid without the addition of any constraints. The avoidance of constraints requires that Lagrange kinematics be employed, either in its complete form, or in the case of steady flow problems, in the truncated form based on streamfunctions. (See Section II D of Paper I.) The principles developed according to this approach are surveyed in subsection A.3 below.

The third approach was inspired by Hargreaves'[25] indication that, in the case of steady compressible flow, the pressure could be made to serve as a Lagrangian density. This idea inspired Bateman[26] to construct a very useful principle for compressible potential flow that will be discussed in subsection A.2 below. There exist two different generalizations[6, 27] of Bateman's principle to rotational baroclinic flow, for both of which the action integral is the space-time integral of the pressure functional.

The fourth approach was introduced by Clebsch.[28] He first effectively integrated Euler's equation by expressing the velocity and pressure (or molar enthalpy in the compressible case) in terms of three new functions ($\varphi$, $\alpha$, and $\beta$) in such a way that, if two of these ($\alpha$ and $\beta$) are constants of motion, Euler's equation is identically satisfied. The

problem then becomes one of finding a variational principle whose Euler–Lagrange equations are the statements that mass (or mole number) is conserved, and that $\alpha$ and $\beta$ are constants of motion. Clebsch constructed such a variational principle for time-dependent incompressible flow. The generalization of this approach to compressible baroclinic flow is embodied in the Seliger-Whitham[27] principle. These two principles are discussed in subsection A.4 below.

The fifth approach[6, 29] to the construction of a variational principle for fluid flow is to attempt a conscious generalization of the classical equilibrium thermodynamical theory of homogeneous systems at rest, i.e. thermostatics, to a true thermodynamics, i.e. a thermodynamical formalism valid for a heterogeneous continuum in an arbitrary state of motion. Such a theory generalizes the thermostatic concept of "equilibrium" to the dynamic concept of fluid flow that obeys the equations of motion. The basic inequality that embodies the Second Law is exploited to construct a representation of non-equilibrium states of motion. This, of course, is the approach of the present paper. Two previous attempts,[6, 29] that were not so closely linked to Hamilton's Principle and did not involve an explicit calculation of the second variation, were carried out in the context of Special Relativity because of the guidance it affords in generalizing a static formalism to one applicable to a system in motion.

It is possible to survey the literature that deals with the second variation of a principle applicable to fluids very quickly, because it is almost non-existent. From the earliest days of the one-dimensional Hamilton's Principle for time-dependent particle motion, it has been recognized that, if the time interval over which the action integral is integrated is short enough, the kinetic energy will dominate the potential energy to such a degree that the second variation will be positive-definite, but for a longer time interval the second

variation becomes indefinite in sign, even though the physical stability of the motion has not been changed in the slightest. The two ends ($t_I$ and $t_F$) of the critical time interval at which the change-over occurs are known as "conjugate points," and the attempt to predict the onset of this change-over has given rise to the so-called "accessory problem."[30] In the multi-dimensional Hamilton's Principle that is relevant to fluid dynamics, the conjugate points become complicated surfaces, and the criterion for locating them in space-time involves solving a complicated set of partial differential equations. In any case, all of this is irrelevant to practical fluid dynamics because it can be taken as axiomatic that, in the case of any problem that is complicated enough to be of interest, the necessary range of integration will be large enough to make the second variation indefinite in sign. Thus the practical need is not for intricate criteria to be applied to the irreducible form of Hamilton's Principle in order to predict the onset of trouble (whose presence can safely be assumed), but rather the need is for different variational principles that avoid the trouble in the first place. A recent investigation[31] of the second variation of the Lin-Rubinov form of Hamilton's Principle for compressible steady flow (discussed in subsection A.3) forces no alteration of any of the above conclusions.

The remainder of this survey will be organized according to the kinematical description used in the variational principle.

### A.2 Principles Using the Euler Description

In the Euler description n and V are treated as independent primitive variables (except for the case of potential flow in which $\mathbf{V} \equiv \nabla\varphi$), and so a constraint must be imposed in order to guarantee that $\tilde{n}$ and $\tilde{\mathbf{V}}$ for the extremal flow satisfy the conservation equation. Lagrange[21] did this for incompressible flow. Bateman[32] did it for compressible flow by adapting Clebsch's[28] principle to the Euler description. In this adaptation, Clebsch's three

functions $\varphi$, $\alpha$, and $\beta$ are Lagrange multipliers. Variation of $\varphi$ leads to the conservation equation, and variation of $\alpha$ and $\beta$ respectively leads to the statements that $\beta$ and $\alpha$ are constants of motion. These two constants of motion characterize what might be termed the "fossil vorticity," i.e. that part of the vorticity that is a retained memory of the initial conditions (as distinct from the part that is generated in regions of baroclinic flow). Bateman's adaptation of Clebsch's principle was limited to barotropic flow. Taub[19] had already removed this limitation in the context of the Lagrange description, and Zilsel,[33] Ito,[34] and Herivel[35] did the same thing in the Euler description. These three authors did not, however, include the term that Bateman had already included that is necessary to describe the fossil vorticity. However, a generalization of this term was re-inserted into the principle as a consequence of C. C. Lin's observation (unpublished, but reported in the review article by Serrin[36]) that, because classical particles maintain their identity, the necessary three identity labels must be constants of motion, and the corresponding constraints together with their Lagrange multipliers should be included in the action integral. This, of course, is all taken care of automatically in the Lagrange description, and is confirmation of the remarks made toward the end of Section I of Paper I regarding the necessity of using the Lagrange description in constructing a variational energy principle.

Two principles for potential flow deserve special mention because despite this limitation they are useful for direct numerical solutions of flow problems. They are the Dirichlet-Kelvin principle for incompressible potential flow and Bateman's[26] generalization of it to compressible potential flow. The **Dirichlet-Kelvin principle** is just the adaptation of the Least Action Principle to the class of trial flows all of which are constrained to be potential flow:

$$\int_V \tfrac{1}{2} n_0 M \mathbf{V} \cdot \mathbf{V} d^3(x) = \text{minimum}; \quad \mathbf{V} \equiv \nabla\varphi \qquad (121a, b)$$

where $n_0$ is the constant density and $\varphi$ is the velocity potential. Bateman's principle says that for subsonic flow

$$\int_V P(H)\, d^3(x) = \text{maximum};\quad H \equiv H^* - \tfrac{1}{2}M(\nabla\varphi)\cdot(\nabla\varphi) \qquad (122a, b)$$

where P(H) is the given pressure function P(H, S) with S suppressed (everywhere the same), and H* is the constant molar stagnation enthalpy. For steady homentropic potential flow with a stagnation enthalpy (Bernoulli constant) that is everywhere the same, Euler's equation is identically satisfied, so the only remaining equation of motion is that of mole conservation, and this is just the Euler-Lagrange equation for the principle given in Equation (122). Bateman showed that the second variation of his action integral is negative-definite if the flow is everywhere subsonic, and indefinite if it is supersonic at any point. This principle has been applied with success[37, 38, 39, 40] to the direct calculation of compressible flow problems.

### A.3 Principles Using the Lagrange Description

As noted at the beginning of Section VI, the first variation of the irreducible form of Hamilton's Principle for time-dependent compressible flow was calculated in the convected frame early on.[16-19] The corresponding calculation in an inertial frame was later carried out by Bretherton[41] without, however, giving an explicit representation (such as Eq. (2c) above) of the velocity as a function of the Lagrange surfaces. In the restricted sense of steady incompressible flow, however, Clebsch[42] long ago developed a principle in which the steady three-dimensional velocity was expressed in terms of two streamfunctions. Clebsch's action integral is

$$\int [\tfrac{1}{2}n_0 M\mathbf{V}\cdot\mathbf{V} + p^*(\psi^1, \psi^2)]\, d^3(x) \qquad (123a)$$

where

$$\mathbf{V} \equiv (\nabla\psi^1 \times \nabla\psi^2)/n_o \qquad (123b)$$

and $n_o$ is the constant density and $p^*(\psi^1, \psi^2)$ is the given stagnation pressure which, because it is a function only of the two streamfunctions $\psi^1$ and $\psi^2$, is a constant of motion. The two functions $\psi^1(\boldsymbol{x})$ and $\psi^2(\boldsymbol{x})$ are the undetermined functions of the problem, and Clebsch showed that the Euler–Lagrange equations corresponding to their variation are equivalent to Euler's equation for steady incompressible flow which can be put into the form $n_o M\ \mathbf{V} \times (\nabla \times \mathbf{V}) = \nabla p^*$. (Because its projection onto V vanishes, it has only two degrees of freedom corresponding to the two variables $\psi^1$ and $\psi^2$.) This 1857 principle of Clebsch has surprisingly been almost completely ignored. (The 1859 principle,[28] which is entirely different, has received much more attention.) The principle given in Equation (123) is valid for three-dimensional **rotational** flow, and for this reason should prove very useful for direct numerical solutions of incompressible steady flow problems with non-zero vorticity.

Bateman[43] gave a principle that is essentially Hamilton's Principle for steady compressible barotropic with the density flux **n** described in terms of a single streamfunction $\psi(x, y)$ and the mole density $n = n(x, y)$ treated as an independent primitive variable. His action integral is

$$\iint [\tfrac{1}{2}M\mathbf{n} \cdot \mathbf{n}/n - u(n)]\, dxdy; \quad \mathbf{n} = \nabla\psi \times \mathbf{e}_z \qquad (124a, b)$$

where $u(n)$ is the given internal energy density. The extremal flow for this principle turns out to be compressible **potential** flow, and as Lush and Cherry[40] pointed out, this principle is a companion piece to the one given in Equation (122) in the sense that, taken together, they constitute a minimax description of subsonic compressible potential flow.

Because entropy has been suppressed in the $u(n)$ that appears in Equation (124a), the flow is barotropic. The Euler–Lagrange equation corresponding to variation of n is $\tilde{H}^* \equiv \tilde{W} + \tilde{H} = 0$. By first suppressing the entropy, and then making the stagnation enthalpy $\tilde{H}^*$ spatially uniform, potential flow must result. This restriction was lifted by Lin and Rubinov[44] who re-inserted the entropy $S = S(\psi)$ as a specified function of the streamfunction (and hence a constant of motion). Their action integral is

$$\iint \{\tfrac{1}{2}M(\mathbf{n} \cdot \mathbf{n}/n) + nH^*(\psi) - u[n, S(\psi)]\}\, dxdy \tag{125}$$

where $\mathbf{n}$ is given by Equation (124b) and $H^*(\psi)$ and $S(\psi)$ are given functions. (They actually restricted themselves to the case $H^* =$ constant.) Besides treating the case of plane flow, they also used the Stokes streamfunction to treat axisymmetric flow. However, the principle is equally valid if $\mathbf{n} \equiv \nabla\psi^1 \times \nabla\psi^2$, $H^* = H^*(\psi^1, \psi^2)$, and $S = S(\psi^1, \psi^2)$. Comparing Equation (125) with Equations (123a) and (124a), it is evident that the Lin–Rubinov principle is a combination of Clebsch's 1857 principle and the Bateman principle of Equation (124) in which $p^*$ of Clebsch's principle has gone over into $nH^*$, and the transition to compressibility requires that $-u(n, S)$ be included in the integrand.

### A.4 Principles Using the Clebsch Description

In an effort to generalize his 1857 principle from steady to unsteady flow Clebsch[28] expressed V in the Pfaffian form

$$\mathbf{V} = \nabla\varphi + \alpha\nabla\beta \tag{126a}$$

and showed that if S is everywhere the same (homentropic flow) and H is defined by

$$\tfrac{1}{2}M\mathbf{V} \cdot \mathbf{V} + H = H^* \tag{126b}$$

where

$$H^* \equiv -[(\partial_t\varphi)_x + \alpha(\partial_t\beta)_x]\,, \tag{126c}$$

then if $\alpha$ and $\beta$ are constants of motion, Euler's equation will be identically satisfied. (Clebsch actually worked with the stagnation and local pressures p* and p rather than with H*, H, and S. These quantities have been introduced in order to facilitate the transition to the Seliger–Whitham principle discussed below.) Using this theorem, Clebsch constructed a variational principle based on the action integral

$$\int_{(V,\Delta t)} n_o [\tfrac{1}{2}M\mathbf{V}\cdot\mathbf{V} - H^*]\, d^3(x)\, dt \tag{127}$$

where V and H* are the functions of $\varphi(\boldsymbol{x}, t)$, $\alpha(\boldsymbol{x}, t)$, and $\beta(\boldsymbol{x}, t)$ that are defined in Equations (126a) and (126c). Variations of these functions lead to Euler–Lagrange equations that are just the conservation equation and the statements that $\beta$ and $\alpha$ are constants of motion.

Bateman[45] generalized this principle by letting $n(\boldsymbol{x}, t)$ be variable and by subtracting the given internal energy density $u(n)$ from the integrand of Equation (127). Thus his action integral is

$$\int_{(V,\Delta t)} [\tfrac{1}{2}nM\mathbf{V}\cdot\mathbf{V} + nH^* - u(n)]\, d^3(x)\, dt \tag{128}$$

where V and H* are still given by Equations (126a) and (126c). (The integrands of Equations (125) and (128) have a superficial similarity, but the definitions of H* and of kinetic energy are entirely different.) Because the entropy is suppressed in $u(n)$, the principle of Equation (128) is limited to barotropic flow. Note that lifting this restriction is not just a matter of replacing $u(n)$ by $u[n, S(\psi^1, \psi^2)]$ because the streamfunctions are not included among the variables of Equation (128).

The appropriate generalization to compressible baroclinic flow was given by Seliger and Whitham.[27] They replaced Equations (126a–c) with

$$\mathbf{V} = \nabla\varphi + \alpha\nabla\beta - S\nabla\theta \tag{129a}$$

$$H \equiv H^* - \tfrac{1}{2}MV \cdot V \tag{129b}$$

where

$$H^* \equiv -[(\partial_t\varphi)_x + \alpha(\partial_t\beta)_x - S(\partial_t\theta)_x], \tag{129c}$$

and pointed out that if $\alpha$ and $\beta$ are constants of motion and $D_t\theta = T$, then Euler's equation will be identically satisfied. (Incidentally, this fact is very transparent in a relativistic context.[46]) Their action integral was defined to be

$$\int_{(V,\,\Delta t)} P(H, S)\, d^3(x)\, dt \tag{129d}$$

where P(H, S) is the known pressure function, H is given by Equation (129b), and the undetermined functions are $\varphi(x, t)$, $\alpha(x, t)$, $\beta(x, t)$, $S(x, t)$, and $\theta(x, t)$. (They actually used the variable $\eta \equiv -\theta$.) Mole density n and temperature T are defined by

$$n \equiv (\partial P/\partial H)_S; \quad T \equiv -\frac{(\partial P/\partial S)_H}{(\partial P/\partial H)_S}. \tag{129e, f}$$

They showed that the Euler-Lagrange equations consist of the conservation equation, the statements that $\tilde{\alpha}$, $\tilde{\beta}$, and $\tilde{S}$ are all constants of motion, and that $\tilde{D}_t\tilde{\theta} = \tilde{T}$.

When P(H, S) goes over into the incompressible limit in the manner illustrated in Section VII C above, the Seliger–Whitham principle goes over into the 1859 Clebsch principle of Equation (127), and thus constitutes its natural generalization from incompressible to baroclinic compressible flow. When $\alpha = S = 0$ and $\partial_t\varphi$ = constant, the Seliger-Whitham principle goes over into the Bateman principle of Equation (122), and so constitutes a generalization of this also.

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## FIGURE CAPTIONS

Figure 1. Virtual Work Performed on a Box of Gas in Deforming its Lagrange Surfaces. (A) Work Performed by an External Energy Source that Produces a Quasi-Static Deformation Against the Internal Pressure p. (B) Work Performed by Spontaneous Conversion of Thermal Energy Within a Small Sample of Gas into Work of Expansion Against the Surrounding Pressure P.

Figure 2. Potential Energy of a Molar "Bubble". (A) Compressive Energy of a Bubble With Molar Volume. (B) Change in Gravitational Energy of a Bubble that Displaces Molar Mass.

Figure 3. (A) Non-Equilibrium Internal Energy Surface $\mathcal{U}(H, \hat{V})$ and its Ridge-Line, the Equilibrium Internal Energy $\tilde{U}(\hat{V})$. (B) Projection of Figure A onto $(\mathcal{U} - \hat{V})$-Plane Showing $\tilde{U}(\hat{V})$ as Boundary of Region of Virtual Fluctuations.